(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
13 September 2001 (13.09.2001)

PCT

(10) International Publication Number
WO 01/66599 A1

(51) International Patent Classification[7]: C07K 14/72

(21) International Application Number: PCT/IB01/00475

(22) International Filing Date: 9 March 2001 (09.03.2001)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
0005689.5 9 March 2000 (09.03.2000) GB

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(81) Designated States *(national)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW.

(84) Designated States *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

Published:
— *with international search report*
— *before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments*

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

WO 01/66599 A1

(54) Title: CRYSTAL

(57) Abstract: A crystal comprising an androgen receptor ligand binding domain (AR-LBD) is provided. The crystal structures of the human Androgen Receptor Ligand Binding Domain (hAR-LBD) in comparison with the human Progesterone Receptor Ligand Binding Domains (hPR-(hPR-LBD) complexed with the same ligand metribolone (R1881) are also provided. The three-dimensional structures of the hAR LBD as well as the hPR LBD show the typical nuclear receptor fold. The change of two residues in the ligand binding pocket (LBP) between hPR and hAR seems to be the most likely source for the specificity of the R1881 ligand binding to hAR LBD. The structural implications of the 14 known mutations in the LBP of the hAR LBD associated with either prostate cancer (PC) or the partial androgen receptor insensitivity syndrome (PAIS) or complete androgen receptor insensitivity syndrome (CAIS) are analysed. The effects of most of these mutants may be explained on the basis of the crystal structure.

CRYSTAL

FIELD OF THE INVENTION

The present invention relates to a crystal structure.

In particular, the present invention relates to a crystal structure for a ligand binding domain (LBD).

In particular, the present invention relates to a crystal structure for a ligand binding domain (LBD) optionally having a ligand which is associated therewith.

In particular, the present invention relates to a crystal structure for a LBD of a receptor.

More in particular, the present invention relates to a crystal structure for a LBD of an androgen receptor (AR-LBD) and also to a crystal structure for an AR-LBD-ligand complex.

The structure may be used to determine androgen receptor homologues and information about secondary and tertiary structures of polypeptides which are as yet structurally uncharacterised. The structure may also be used to identify ligands which are capable of binding to the androgen receptor. Such ligands may be capable of acting as modulators of androgen receptor activity.

The crystal structure of AR-LBD enables a model to be produced for androgen receptor activity. Thus, the present invention provides a model which can be used to understand the structural implications of the binding mechanism.

BACKGROUND TO THE INVENTION

The androgen receptor (AR) is a member of the superfamily of nuclear receptors which includes, amongst others, the steroid receptors as well as the vitamin D, thyroid, retinoic acid receptors and the so-called orphan receptors. In addition, the AR is a member of a group of four closely related steroid receptors including the progesterone receptors (PR), the mineralocorticoid receptor and the glucocorticoid receptor all of which recognise the same hormone response element. In general, steroid receptors are comprised of five to six domains which act as ligand-activated transcription factors that control the expression of specific genes. The ligand binding region is located in the C terminal domain and is called the ligand binding domain (LBD). Binding of a ligand (such as a steroid hormone) to the LBD induces changes in receptor conformation that control transcriptional activation and repression and also regulate homo- or heterodimerisation. In the absence of ligand, these receptors repress basal gene expression, probably through the expression of co-repressor proteins.

The androgen hormones and their receptors play an important role in male physiology and pathology. The androgen receptor binds the male sex steroids, dihydrotestosterone (DHT) and testosterone [Teutsch, 1994], and regulates genes for male differentiation and development. Consequently, constitutional mutations in the androgen receptor gene may lead to several disease states. Some examples of these diesease states include prostate cancer (PC) and the androgen insensitivity syndrome (AIS) which are capable of impairing androgen-dependent male sexual differentiation to various degrees. In addition, complete androgen insensitivity syndrome (CAIS) leads to an unequivocally external female phenotype. In contrast, partial or incomplete androgen insensitivity syndrome (PAIS) comprises a wide spectrum of clinical phenotypes while mild androgen insensitivity syndrome (MAIS), is connected to forms of undervirilisation [Bellis, 1992]. About 50% of the mutated residues reported in the human androgen receptor ligand binding domain (hAR LBD) to date are found to be involved in

prostate cancer (PC) and in AIS [Gottlieb, 1998]. These mutations have been well documented in the Androgen Receptor Gene Mutations Database of the Lady Davis Institute for Medical Research [Gottlieb, 1998].

To date, there are a total of 20 known amino acid residues in the AR LBD which are involved in ligand interaction. Of these 20 amino acid residues, to date, mutations have been reported in 14 of the 20 amino acid residues. These mutations are largely in the ligand binding pocket (LBP) which is part of the AR-LBD. By way of example, the three mutations in the LBP of the hAR , which have been described for CAIS, these being N705S [Bellis, 1992; Pinsky, 1992], L707R [Lumbroso, 1996] and M749V [Bellis, 1992; Jakubicza, 1992]} are recognised as substitutions that considerably change the size and charge properties of the respective amino acid side chains. However, while it is known that these amino acid substitutions result in a considerably change in size of the respective amino acid side chains, it is not known how this change in size alters the AR-LBD such that the local structure and interactions with the ligand are disturbed. Moreover, because both the structural implications and the effects of these known mutation have not been determined, no ligand binding data are available for many of the published mutations in the AR-LBD.

In order to develop an understanding of the structural implications of mutations resulting in amino acid substitutions in the AR-LBD, attempts have been made by workers to determine the primary, secondary and tertiary structures of the AR-LBD. In this regard, the LBDs of the different nuclear receptor families have been analysed and shown to share a similar fold in spite of their low (about 20%) sequence homology. In this respect, the receptor fold has been shown to comprise about 12 helices and several small β-sheet arranged in a so-called "α-helical sandwich". Up until now, this kind of fold has only been observed for the LBDs of nuclear receptors. However, it has also been shown that, depending on the nature of the bound ligand, which may be an agonist or an antagonist, the carboxyterminal helix H12 may be found in either one of two orientations. In the

agonist-bound conformation, helix H12 serves as a 'lid' to close the ligand-binding pocket (LBP), which contains the LBD, whereas in the antagonist-bound conformation, helix H12 is positioned in a different orientation thus opening the entrance to the LBP.

Despite the availability of information regarding the role of the helix H12 region in ligand binding, there is very little experimental information available about the structure or the role of the other helical regions (such as helices H1 to H11) with respect to ligand binding. By way of example, there has been a suggestion that helices H4 and H5 may be regions involved in ligand binding. However, no experimental information is available with respect to these helices in the AR-LBD. In addition, while it is thought that while about 50% of the mutated residues reported in the hAR LBD are found to be involved in prostate cancer (PC) and in AIS [Gottlieb, 1998], it is not known experimentally whether the mutations are predominantly found in the interior of the receptor protein or at the surface of the receptor protein.

Structurally, it is known that the nuclear receptors, such as the androgen receptor, can be organised into functional modules comprising an N-terminal transcriptional activation domain, a central DNA binding domain (DBD) and a C-terminal ligand binding domain (LBD). During the past few years, X-ray structures have been published for two of the domains, the DNA-binding domain as well as for a number of ligand-binding domains (LBD) including LBD-ligand complexes of receptors such as the estrogen receptor α and β, the progesterone receptor (PR), the vitamin D receptor, the retinoic acid receptors (X: RXR, acid: RAR), the thyroid hormone receptor and the peroxisome proliferator-activated receptors [Moras, 1998; Brzozowski, 1997; Tannenbaum, 1998; Shiau, 1998; Bourguet, 1995; Renaud, 1995; Wagner, 1995; Ribeiro, 1998; Williams, 1998; Nolte, 1998; Uppenberg, 1998 ; Klaholz, 1998; Rochel, 1999].

To date, no X-ray structures have been published for the AR-LBD either alone or in combination with a ligand. Although a model structure of the AR-LBD has been developed by Yong et al (1998), this model is based on the crystal structure of the RARα LBD [Bourguet, 1995] and not on either the AR-LBD or a more closely related receptor such as a PR-LBD. In addition, no experimentally determined three-dimensional (3D) structure is available for a complete androgen receptor either alone or in combination with a ligand. Furthermore, although the crystal structure of the progesterone receptor (PR) LBD in complex with progesterone was published in 1998 by Williams and Sigler, no comparative experimental analyses have been carried out between closely related steroid receptors such as an androgen receptor-LBD and progesterone receptor, either alone or complexed with ligands in order to identify ligand specificities and/or ligand specific residues.

SUMMARY OF THE INVENTION

In a broad aspect the present invention relates to cystal structures of receptor ligand binding domains including the uses thereof.

SUMMARY ASPECTS

According a first aspect of the invention there is provided a crystal structure comprising an AR-LBD.

In a preferred embodiment the crystal structure is a crystal structure for an AR-LBD.

The structure of a crystal AR-LBD has been solved and is set forth in Table 4.

In a second aspect the present invention provides a crystal structure comprising an AR-LBD-ligand complex.

In a third aspect the present invention provides a crystal structure comprising an AR-LBP.

According to a fourth aspect of the invention, there is provided a model of at least part of an AR-LBD made using or comprising or depicting a crystal structure according to any one of the first, second and third aspects of the invention. The crystal structure of the first, second and third aspect of the invention and the model of the fourth aspect of the invention may be provided in the form of a computer readable medium.

The crystals and models of earlier aspects of the invention may provide information about the atomic contacts involved in the interaction between the receptor and a known ligand, which can be used to screen for unknown ligands.

According to a fifth aspect of the invention, there is provided a method of screening for a ligand capable of binding an androgen receptor binding domain, comprising the use of a crystal structure according to any one of the first, second or third aspects of the invention or a model according to the fourth aspect of the invention. For example, the method may comprise the step of contacting the AR-LBD with a test compound, and determining if said test compound binds to said ligand binding domain. The method may be an *in vitro* method and/or an *in silico* method and/or an *in vivo* method.

In a sixth aspect, the present invention provides a ligand identified by a screening method of the fifth aspect of the invention. Preferably the ligand is capable of modulating the activity of an AR-LBD. As mentioned above, ligands which are capable of modulating the activity of AR-LBDs have considerable therapeutic and prophylactic potential.

In a seventh aspect, the present invention provides the use of a ligand according to the sixth aspect of the invention, in the manufacture of a medicament to treat and/or prevent a disease in a mammalian patient. There is also provided a pharmaceutical composition comprising such a ligand and a method of treating and/or preventing a disease comprising administering the step of administering such a ligand according or pharmaceutical composition to a mammalian patient.

The crystal structures and models described above also provide information about the secondary and tertiary structure of AR-LBDs. This can be used to gleen structural information about other, previously uncharacterised polypeptides. Thus, according to an eighth aspect of the invention there is provided a method of determining the secondary and/or tertiary structures of polypeptides with unknown (or only partially known) structure comprising the step of using such a crystal or model. The polypeptide under investigation is preferably structurally or functionally related to the androgen receptor ligand binding domain. For example, the polypeptide may show a degree of homology over some or all parts of the primary amino acid sequence. Alternatively, the polypeptide may perform an analogous function or be suspected to show a similar binding mechanism to the AR-LBD.

The present invention demonstrates that the hAR-LBD crystal structure can be used to analyse and explain the structural implications of 14 known mutations in the LBP of the hAR LBD which are associated with either prostate cancer (PC), the partial androgen receptor insensitivity syndrome (PAIS), mild androgen receptor insensitivity syndrome (MAIS) or complete androgen receptor insensitivity syndrome (CAIS).

The present invention also demonstrates that a crystal structure of an AR-LBD may be used to identify ligands (such as agonists/antagonists) with binding specificity for the AR LBD. In this way, compounds may be selected, improved or modified to improve this ligand binding interaction.

The present invention also provides the crystal structure of the human hAR LBD in complex with the ligand metribolone (R1881) and the crystal structure of the human hPR LBD in complex with the ligand metribolone (R1881). The provision, for the first time, of these two experimentally determined three dimensional (3D) crystal stuctures has facilitated a comparison to be drawn between the crystal structure of both receptors in complex with the same ligand. Up until now, it has been known from studies on model receptros that the AR-LBD and the PR-LBD have a number of similarities in that:

(i) they belong to the same steroid receptor subfamily;

(ii) they share about 54% LBD sequence identity (Figure 1); and

(iii) there are a number of different ligands with similar binding affinities for both receptors [Teutsch, 1994].

The present invention highlights an additional similarity between the hAR-LBD and hPR-LBD ligand complexes in that the three-dimensional structures of the hAR LBD as well as the hPR LBD demonstrate the typical nuclear receptor fold.

The present invention also demonstrates some hitherto unknown, but important, differences between the two receptors. These include:

(i) the identification of a two amino acid residue change in the ligand binding pocket (LBP) of the AR-LBD which is the most likely site for the specific binding of the R1881 ligand to the hAR-LBD. The AR-LBD amino acid residues are Leu 880 and Thr 877. The corresponding PR-LBD amino acid residues are Thr 894 and Cys 891. In addition, there are three other amino acid changes which maybe involved in binding of ligands other than R1881. The AR amino acid residues are

Gln 783, Met 749 and Phe 876. The PR amino acid residues are Leu 797, Leu 763 and Tyr 890.

(ii) the demonstration that the hPR LBD – R1881 complex crystallises as a dimer in the asymmetric unit whereas the hAR LBD-R1881 complex crystallises as a monomeric unit.

(iii) the demonstration that the two independent molecules in the crystal structure of hPR LBD - R1881 exhibit different modes of ligand binding. One orientation of R1881 in one monomer resembles that of R1881 in the hAR LBD complex, while in the second monomer, R1881 is orientated similar to progesterone in the hPR LBD – progesterone complex.

The present invention demonstrates the surprising and unexpected findings that:

(i) the helix H6 in the AR-LBD is an α-helix. In striking contrast, no α-helix was found either in the model hAR-LBD in this area or in the hPR-LBD-progesterone complex (Molecule A) (see Figure 4) whereas in the hPR-LBD-progesterone complex (Molecule B), an α-helix is observed.

(ii) helices H4 and H5 and helices H10 and H11 are preferably contiguous helices. That is, these helices H4 and H5 and H10 and H11 are connected to each other to form 2 continuous helices rather than 4 separate helices. Accordingly, the α-helical sandwich structure for the AR-LBD comprises preferably 9 α-helical regions instead preferably 11 α-helices. This observation was not seen in the liganded PR-LBD (Williams, 1998) which comprises 10 α-helices and where only helices H10 and H11 are contiguous sequences.

(iii) in the hAR-LBD-R1881 complex, the helix H12 is split into two shorter helical segments with 9 and 5 amino acid residues respectively. This observation

was not seen in the hPR LBD-R1881 complex structure although a bending of helix H12 was also seen. As it is known that helix H12 may influence the binding of antagonists and agonists, this finding may have important implications for ligand binding.

(iv) the demonstration that the two independent molecules in the crystal structure of hPR LBD - R1881 exhibit different modes of ligand binding. One orientation of R1881 in one monomer resembles that of R1881 in the hAR LBD complex, in the second monomer R1881 is orientated similar to progesterone in the hPR LBD – progesterone complex.

The present invention is advantageous as the determination of the 3D structure of the AR-LBD allows the AR-LBD to be mapped.

The use of the crystals stucture in conjunction with this map enables a better understanding of ligand specificities for the AR-LBD.

In particular, the crystal structure of the present invention now makes it possible to see:

(i) not only how a ligand binds to the AR-LBD but also

(ii) the structural reasons why a ligand binds to an AR-LBD.

Using the crystal structure, these effects can not only be understood but can also be predicted. This improved understanding of the AR-LBD facilitates the identification and modification of ligands which are capable of specifically and/or preferentially interacting with the AR-LBD.

The present invention is also advantageous as it facilitates:

(i) the identification and characterization of the key residues within the AR-LBD and a comparison with those associated with the PR-LBD. In this regard, the present invention demonstrates an important new finding in relation to the PR-LBD-progesterone complex. In this respect, Asn 705 in the AR-LBD and Asn 719 in the PR-LBD have been shown to be capable of acting as hydrogen bond partners for ligands, which have, for example, a hydroxyl group attached to position 17 or to a substituent attached to position 17 on a steroidal ligand.

(ii) the identification and characterization of the interaction of ligands with the AR-LBD sites.

(iii) the identification of ligands with enhanced properties capable of interacting with one or more residues of the LBD. These enhanced properties include but not limited to: (a) higher affinity, (b) improved selectivity for the AR, and/or (c) a designated degree of efficacy (agonism vs. partial agonism vs. antagonism vs partial antagonism).

(iv) the design of one or more ligands which may specifically bind to an AR-LBD but not to a PR-LBD (ie a selective ligand).

(v) the determination of the structural effects associated with a mutation. (In this respect, although, many of the phenotypic traits associated with the characterised mutations in the androgen receptor gene are known, the structural implications of such mutations have not been determined).

(vi) the identification of ligands capable of overcoming the mutation/structural disturbance in the AR-LBD and/or LBP comprising the AR-LBD.

(vii) the determination of ligand binding data (affinity constants etc) which have not been available for many of the published mutant receptors.

(viii) the implementation of an iterative drug design and/or for "reverse-engineering" or " *de novo* design" of compounds and/or "structure-based drug design".

(ix) a detailed understanding of the structure of the LBDs receptors, such as the AR and PR which enables *in vitro* ligand binding data to be explained and understood.

(x) a reduction in the length of time required to discover compounds that target the AR-LBD.

Other aspects of the present invention are presented in the accompanying claims and in the following description and drawings. These aspects are presented under separate section headings. However, it is to be understood that the teachings under each section are not necessarily limited to that particular section heading.

DETAILED ASPECTS OF THE INVENTION

Unless otherwise indicated, all terms used herein have the same meaning as they would to one skilled in the art of the present invention. Practitioners are particularly directed to Current Protocols in Molecular Biology (Ansubel) for definitions and terms of the art.

According to one aspect of the present invention, there is provided a crystal structure comprising an androgen receptor ligand binding domain (AR-LBD).

Preferably the AR-LBD is a human AR-LBD.

In a preferred aspect of the present invention, there is provided a crystal structure comprising a ligand binding domain (LBD) wherein the LBD is arranged in an α-helical sandwich comprising preferably the α-helices H1, H3, H4, H5, H6, H7,

H8, H9, H10, H11 and H12; preferably two 3_{10} helices; and preferably four short β strands (S1, S2, S3 and S4) associated in two anti-parallel β-sheets; wherein the helices H4, H5, H10 and H11 are preferably contiguous helices; and wherein either helix H6 is preferably an α-helix and/or helix H12 comprises preferably two helical segments of preferably 9 amino acid residues and preferably 5 amino acid residues.

CRYSTAL

As used herein, the term "crystal" means a structure (such as a three dimensional (3D) solid aggregate) in which the plane faces intersect at definite angles and in which there is a regular structure (such as internal structure) of the constituent chemical species. Thus, the term "crystal" can include any one of: a solid physical crystal form such as an experimentally prepared crystal, a 3D model based on the crystal structure, a representation thereof such as a schematic representation thereof or a diagrammatic representation thereof, a data set thereof for a computer.

CRYSTAL PREPARATION

The crystals of the present invention may be prepared by expressing a nucleotide sequence encoding the AR-LBD and PR-LBD by use of a suitable host cell and then crystallising the purified receptor protein.

The invention also features a method for creating crystalline AR-LBD structures described herein. The method may utilize a polypeptide comprising an AR-LBD described herein to form a crystal. A polypeptide used in the method may be chemically synthesized in whole or in part using techniques that are well-known in the art. Alternatively, methods are well known to the skilled artisan to construct expression vectors containing the native or mutated AR-LBD coding sequence and appropriate transcriptional/translational control signals. These

methods include *in vitro* recombinant DNA techniques, synthetic techniques, and *in vivo* recombination/genetic recombination. See for example the techniques described in Sambrook et al. (Molecular Cloning: A Laboratory Manual, 2nd Edition, Cold Spring Harbor Laboratory press (1989)), and other laboratory textbooks. (See also Sarker et al, Glycoconjugate J. 7:380, 1990; Sarker et al, Proc. Natl. Acad, Sci. USA 88:234-238, 1991, Sarker et al, Glycoconjugate J. 11: 204-209, 1994; Hull et al, Biochem Biophys Res Commun 176:608, 1991 and Pownall et al, Genomics 12:699-704, 1992).

Crystals are grown from an aqueous solution containing the purified AR-LBD polypeptide by a variety of conventional processes. These processes include batch, liquid, bridge, dialysis, vapor diffusion, and hanging drop methods. (See for example, McPherson, 1982 John Wiley, New York; McPherson, 1990, Eur. J. Biochem. 189: 1-23; Webber. 1991, Adv. Protein Chem. 41:1-36). Generally, the native crystals of the invention are grown by adding precipitants to the concentrated solution of the AR-LBD polypeptide. The precipitants are added at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

Derivative crystals of the invention can be obtained by soaking native crystals in a solution containing salts of heavy metal atoms. A complex of the invention can be obtained by soaking a native crystal in a solution containing a compound that binds the AR-LBD, or they can be obtained by co-crystallizing the AR-LBD polypeptide in the presence of one or more compounds that bind to the AR-LBD.

Once the crystal is grown it can be placed in a glass capillary tube and mounted onto a holding device connected to an X-ray generator and an X-ray detection device. Collection of X-ray diffraction patterns are well documented by those skilled in the art (See for example, Ducruix and Geige, 1992, IRL Press, Oxford, England). A beam of X-rays enter the crystal and diffract from the crystal. An X-

ray detection device can be utilized to record the diffraction patterns emanating from the crystal. Suitable devices include the Marr 345 imaging plate detector system with an RU200 rotating anode generator.

Methods for obtaining the three dimensional structure of the crystalline form of a molecule or complex are described herein and known to those skilled in the art (see Ducruix and Geige). Generally, the x-ray crystal structure is given by the diffraction patterns. Each diffraction pattern reflection is characterized as a vector and the data collected at this stage determines the amplitude of each vector. The phases of the vectors may be determined by the isomorphous replacement method where heavy atoms soaked into the crystal are used as reference points in the X-ray analysis (see for example, Otwinowski, 1991, Daresbury, United Kingdom, 80-86). The phases of the vectors may also be determined by molecular replacement (see for example, Naraza, 1994, Proteins 11:281-296). The amplitudes and phases of vectors from the crystalline form of an AR-LBD determined in accordance with these methods can be used to analyze other crystalline AR-LBDs.

The unit cell dimensions and symmetry, and vector amplitude and phase information can be used in a Fourier transform function to calculate the electron density in the unit cell i.e. to generate an experimental electron density map. This may be accomplished using the PHASES package (Furey, 1990). Amino acid sequence structures are fit to the experimental electron density map (i.e. model building) using computer programs (e.g. Jones, TA. et al, Acta Crystallogr A47, 100-119, 1991). This structure can also be used to calculate a theoretical electron density map. The theoretical and experimental electron density maps can be compared and the agreement between the maps can be described by a parameter referred to as R-factor. A high degree of overlap in the maps is represented by a low value R-factor. The R-factor can be minimized by using computer programs that refine the structure to achieve agreement between the theoretical and

observed electron density map. For example, the XPLOR program, developed by Brunger (1992, Nature 355:472-475) can be used for model refinement.

A three dimensional structure of the molecule or complex may be described by atoms that fit the theoretical electron density characterized by a minimum R value. Files can be created for the structure that defines each atom by coordinates in three dimensions.

AR AND PR CONSTRUCTS

The proteins comprising the AR-LBD and PR-LBD may be produced by a host recombinant cell may be secreted or may be contained intracellularly depending on the nucleotide sequence and/or the vector used. As will be understood by those of skill in the art, expression vectors containing the AR and PR encoding nucleotide sequences can be designed with signal sequences which direct secretion of the AR and PR coding sequences through a particular prokaryotic or eukaryotic cell membrane. Other recombinant constructions may join the AR or PR encoding sequence to nucleotide sequence encoding a polypeptide domain which will facilitate purification of soluble proteins (Kroll *DJ et al* (1993) DNA Cell Biol 12:441-53). Such purification facilitating domains include, but are not limited to, metal chelating peptides such as histidine-tryptophan modules that allow purification on immobilized metals (Porath J (1992) Protein Expr Purif 3 - .26328 1), protein A domains that allow purification on immobilized immunoglobulin, and the domain utilized in the FLAGS extension/affinity purification system (Immunex Corp, Seattle, WA). The inclusion of a cleavable linker sequence such as Factor XA or enterokinase (Invitrogen, San Diego, CA) between the purification domain and the AR and PR is useful to facilitate purification.

HOST CELLS

A wide variety of host cells can be employed for expression of the nucleotide sequences encoding the AR and PR proteins of the present invention. These cells may be both prokaryotic and eukaryotic host cells. Suitable host cells include bacteria such as *E. coli*, yeast, filamentous fungi, insect cells, mammalian cells, typically immortalized, e.g., mouse, CHO, human and monkey cell lines and derivatives thereof. Preferred host cells are able to process the expression products to produce an appropriate mature polypeptide. Processing includes but is not limited to glycosylation, ubiquitination, disulfide bond formation and general post-translational modification.

NUCLEOTIDE SEQUENCES

As used herein, the term "nucleotide sequence" refers to nucleotide sequences, oligonucleotide sequences, polynucleotide sequences and variants, homologues, fragments and derivatives thereof (such as portions thereof) which comprise the nucleotide sequences encoding the AR-LBD and PR-LBD. The nucleotide sequence may be DNA or RNA of genomic or synthetic or recombinant origin which may be double-stranded or single-stranded whether representing the sense or antisense strand or combinations thereof. Preferably, the term nucleotide sequence is prepared by use of recombinant DNA techniques (e.g. recombinant DNA). The nucleotide sequence may include within them synthetic or modified nucleotides. A number of different types of modification to oligonucleotides are known in the art. These include methylphosphonate and phosphorothioate backbones, addition of acridine or polylysine chains at the 3' and/or 5' ends of the molecule. For the purposes of the present invention, it is to be understood that the nucleotide sequences described herein may be modified by any method available in the art. Such modifications may be carried out in order to enhance the *in vitro* activity or life span of nucleotide sequences of the invention.

Preferably, the term "nucleotide sequence" means cDNA.

FUSION PROTEINS

The AR and PR proteins comprising the AR-LBD and PR-LBD of the present invention may also be produced as fusion proteins, for example to aid in extraction and purification. Examples of fusion protein partners include glutathione-S-transferase (GST), 6xHis, GAL4 (DNA binding and/or transcriptional activation domains) and β-galactosidase. It may also be convenient to include a proteolytic cleavage site between the fusion protein partner and the protein sequence of interest to allow removal of fusion protein sequences.

AMINO ACID SEQUENCES

Preferably the fusion protein will not hinder the ligand binding activity of the AR-LBD and PR-LBD comprising the amino acid sequences (SEQ ID No 1 and SEQ ID No 3 respectively) of the present invention.

Preferably AR-LBD comprises at least SEQ ID No 1, or a homologue or mutant thereof.

Preferably the PR-LBD comprises at least SEQ ID No 3, or a homologue or mutant thereof.

CRYSTALLISATION

After cleavage of the fusion protein, the AR-LBD and PR-LBD may be separated from the cleavage products by chromatographic methods. Concentration may be performed with the aid of a filtration system and the protein concentrate may be immediatedly used for crystallisation purposes. The protein concentrate may be

crystallised using, for example, the vapour diffusion method at a temperature of from about 1°C to about 30°C, preferably from about 4°C to about 20°C. The crystallisation temperature is dependent on the additives present in the protein solution.

Typically, the crystals comprising the AR-LBD are purified to homogeneity for crystallisation. Purity of the AR-LBDs may be measured by typical techniques such as with SDS-PAGE, mass spectrometry and hydrophobic HPLC.

Preferably crystal comprises the AR-LBD or a homologue or mutant thereof.

Preferably the crystal comprises the PR-LBD or a homologue or mutant thereof.

Preferably the crystal is usable in X-ray crystallography techniques. Preferably the crystals used can withstand exposure to X-ray beams used to produce a diffraction pattern data necessary to solve the X-ray crystallographic structure.

Preferably the crystal has a resolution determined by X-ray crystallography of from about 1.5Å to about 3.5Å, preferably about 1.5Å.

Preferably the crystal has a resolution determined by X-ray crystallography of from about 1.5Å to about 3.0 Å.

Preferably the crystal comprising the AR-LBD has the secondary structure presented as SEQ ID No 2, or a homologue or mutant thereof.

The crystal may be formed from an aqueous solution comprising a purified polypeptide comprising an AR-LBD.

The term "purified" in reference to a polypeptide, does not require absolute purity such as a homogenous preparation rather it represents an indication that the

polypeptide is relatively purer than in the natural environment. Generally, a purified polypeptide is substantially free of other proteins, lipids, carbohydrates, or other materials with which it is naturally associated, preferably at a functionally significant level for example at least 97.5% pure, more preferably at least 99% pure, most preferably at least 99.5% pure. A skilled artisan can purify a polypeptide comprising an AR-LBD using standard techniques for protein purification. A substantially pure polypeptide comprising an AR-LBD will yield a single major band on a non-reducing polyacrylamide gel. The purity of the AR-LBD can also be determined by amino-terminal amino acid sequence analysis.

The term "associate", "association" or "associating" refers to a condition of proximity between a moiety (i.e. chemical entity or compound or portions or fragments thereof), and an AR-LBD, or parts or fragments thereof (e.g. binding sites or domains). The association may be non-covalent i.e. where the juxtaposition is energetically favored by for example, hydrogen-bonding, van der Waals, or electrostatic or hydrophobic interactions, or it may be covalent.

ANDROGEN

As used herein, the term "androgen refers to any substance, natural or synthetic, that is able to stimulate the development of male sexual characteristics. Naturally occuring androgens are represented by the C_{19}-steroid hormones. They are produced especially by the testis (such as testosterone) and also by the adrenal cortex, ovary and the placenta. As used herein, the term "androgen" relates to the male sex steroids, dihydrotestosterone (DHT) and testosterone [Teutsch, 1994] which bind to the AR-LBD and which regulate the genes for male differentiation and development.

ANDROGEN RECEPTOR

As used herein, the term "androgen receptor (AR)" means any of the androgen-binding nuclear proteins that mediate the effects of androgens by regulating gene expression. The androgen receptor proteins are discrete zinc-finger proteins which bind discrete DNA sequences, located upstream of transcriptional start sites, when an AR-ligand complex is formed. The androgen receptor (AR) binding domain, also known as the androgen receptor ligand binding domain (AR-LBD), or the hormone binding domain (HBD), is in the C-terminal region. In humans, a number of variants are known that are associated with abnormalities, including prostate cancer (PC), testicular feminisation syndrome, complete androgen insensitivity syndrome (CAIS) and/or partial androgen insensitivity syndrome (PAIS) and/or mild androgen insensitivity syndrome (MAIS) which may lead to external genitalia varying between female and nearly normal male.

As used herein, the term "androgen receptor" means the wild type androgen receptor or a mutant androgen receptor.

WILD TYPE

The term "wild type" refers to the phenotype that is characteristic of most of the members of a species occuring naturally and which contrasts with the phenotype of a mutant species. As used herein, the term "wild type androgen receptor" refers to the an androgen receptor comprising the amino acid sequence presented as SEQ ID No 1. In particular, the term "wild type androgen receptor" refers to the androgen receptor comprising a ligand binding pocket (LBP) wherein the LBP is defined by the structural co-ordinates of the AR-LBD amino acid residues L701; L704; N705; L707; Q711; M742; L744; M745; M749; R752; F764; Q783; M787; F876; T877; L880; F891; M895 or a homologue thereof.

MUTANT

As used herein, the term "mutant" refers to any organism that has undergone mutation or that carries a mutant gene that is expressed in the phenotype of that organism. A mutation may arise due to a substitution of one nucleotide for another or from a deletion of a nucleotide or an insertion of a nucleotide relative to a referenced wild type sequence. These single nucleotide variations are sometimes referred to as single nucleotide polymorphisms (SNPs). Some SNPs may occur in protein-coding sequences, in which case, one of the polymorphic forms may give rise to the expression of a defective or other variant protein and, potentially, a genetic disease. Other SNPs may occur in noncoding regions. Some of these polymorphisms may also result in defective protein expression (e.g., as a result of defective splicing). Other SNPs may have no phenotypic effects.

As used herein, the term "mutant" refers to an androgen receptor comprising any one or more changes in the sequence (and/or the structural co-ordinates) and of the amino acid residues in the AR-LBD which interact with bound ligand wherein the amino acid changes in the AR-LBD may be selected from any one or more of the group of LBD amino acid residues substitutions consisting of:L701H; M749I; T877A; T877S; L880Q; F891L;N705S; L707R; M749V; G708A; G708V; M742V; M742I; M745T; V746M; R752Q; F764S; M787V. In this regard, the sequence and amino acid residues (such as L701H) are described using the one letter format for the amino acid residue (such as L), followed by the amino acid designations nunber which refers to the amino acid residue in the wild type sequence directly above the last digit, followed by the mutant amino acid residue (here a substituted amino acid residue) which is also described using the one letter format for the amino acid residue (in this case H).

For some embodiments the androgen receptor may comprise two or more mutated amino acid residues. An example of such an embodiment is L701H and T877A.

The term "mutant" is not limited to the above mutations which are reflected in amino acid substitutions of the key amino acid residues in the AR-LBD but may also include and is not limited to other deletions or insertions of nucleotides in the wild type sequence which may result in changes in the amino acid residues in the deduced amino acid sequence of the AR-LBD. The term "mutant" also includes uncharacterised mutants.

Preferably the mutated androgen receptor comprises one or more of the characterised mutations in the LBP of the AR-LBD as set out in Table 3.

Preferably the mutated amino acid residue(s) is/are located in helices H4 and H5 of the AR-LBD.

Preferably the mutated amino acid residue(s) is/are evenly distributed between buried, medium and fully accessible amino acid residues within the ligand binding pocket (LBP) comprising the AR-LBD.

Preferably the mutated amino acid residue(s) is/are distributed as set out in Figure 1.

STRUCTURAL CO-ORDINATES

In a highly preferred embodiment, the crystal has the structural co-ordinates as provided in Table 4 (Figure 6) which may be used for the identification of a ligand capable of binding to the AR-LBD.

As used herein, the term "structural co-ordinates" refer to a set of values that define the position of one or more amino acid residues with reference to a system of axes. The term refers to a data set that defines the three dimensional structure of a molecule or molecules (e.g. Cartesian coordinates, temperature factors, and occupancies). Structural coordinates can be slightly modified and still render nearly identical three dimensional structures. A measure of a unique set of structural coordinates is the root-mean-square deviation of the resulting structure. Structural coordinates that render three dimensional structures (in particular a three dimensional structure of an SGC domain) that deviate from one another by a root-mean-square deviation of less than 5 Å, 4 Å, 3 Å, 2 Å, or 1.5 Å may be viewed by a person of ordinary skill in the art as very similar.

According to one aspect of the present invention, there is provided a crystal comprising a complex between an androgen receptor ligand-binding domain and a ligand. In other words the androgen receptor ligand binding domain may be associated with a ligand in the crystal. The ligand may be any compound which is capable of interacting stably and specifically with the androgen receptor ligand binding domain. The ligand may, for example, be an inhibitor of the AR-LBD.

LIGAND-BINDING DOMAIN

As used herein, the term "ligand binding domain (LBD)" means the C-terminal ligand binding region of a steroid receptor which is responsible for ligand binding. The term "ligand binding domain (LBD)" also includes a homologue of the ligand binding domain or a portion thereof. The LBD of the present invention comprises a ligand binding pocket (LBP).With reference to the crystal of the present invention residues in the LBD may be defined by their spatial proximity to the ligand in the crystal structure. The term "ligand binding domain (LBD)" also includes a homologue of the ligand binding domain or a portion thereof.

As used herein, the term "portion thereof" means the structural co-ordinates corresponding to a sufficient number of amino acid residues of AR-LBD (or homologues thereof) that are capable of interacting with a test compound capable of binding to the LBD. This term includes AR- ligand binding domain amino acid residues having an amino acid residues from about 4Å to about 5Å of a bound compound or fragment thereof. Thus, for example, the structural co-ordinates provided in the crystal structure may contain a subset of the amino acid residues in the LBD which may be useful in the modelling and design of compounds that bind to the LBD.

The ligand binding domain may be defined by its association with the ligand.

Preferably the ligand binding domain comprises one or more amino acid residues as determined from the crystal structure or a homologue thereof. Examples of such amino acid residues are presented herein.

LIGAND BINDING POCKET (LBP)

According to one aspect of the present invention, there is provided a crystal structure comprising a ligand binding pocket (LBP); wherein the LBP is defined by the following amino acid residue structural co-ordinates: L701; L704; N705; L707; Q711; M742; L744; M745; M749; R752; F764; Q783; M787; F876; T877; L880; F891; M895; or a homologue thereof.

As used herein, the term “ligand binding pocket (LBP)” refers to the cavity or hollow in a structure – typically a three-dimensional (3D) structure - in which a ligand binds and in which is located the ligand binding domain (LBD). The LBP is sometimes referred to as a “binding niche”. In particular, preferaby, the term AR-LBP refers to the 18-20 known amino acid residues in the hAR-LBD which are known to interact with bound ligand (either R1881 or progesterone). These residues are highlighted in Figure 1 and included in Figure 4. Most of these

residues are hydrophobic and interact mainly with the steroid scaffold, while a few are polar and may form hydrogen bonds to the polar atoms in the ligand.

POLAR AMINO ACIDS

As used herein, the term "polar" includes positively and negatively charged amino acids. In this respect, negatively charged amino acids include aspartic acid (D) and glutamic acid (E); positively charged amino acids include lysine (K) and arginine (R); and amino acids with uncharged polar head groups having similar hydrophilicity values include leucine (L), isoleucine (I), valine (V), glycine (G), alanine (A), asparagine (N), glutamine (Q), serine (S), threonine (T), phenylalanine (F), and tyrosine (Y). The classification of these amino acid residues is set out in the Table below.

HOMOLOGUE

As used herein, the term "homologue" refers to an AR-LBD or a portion thereof which may have deletions, insertions or substitutions of amino acid residues as long as the binding specificity of the AR-LBD is retained. In this regard, deliberate amino acid substitutions may be made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity, and/or the amphipathic nature of the residues as long as the binding specificity of the AR-LBD is retained. Here, a conservative substitution which may produce a silent change which may result in a functionally equivalent AR-LBD.

As used herein, the term "homologue" also means a homologue of the crystal structure of the AR-LBD wherein the homologue has a root mean square (r.m.s) deviation from the backbone atoms of amino acid residues in secondary structural elements of less than 3.0Å. Preferably the r.m.s deviation from the backbone atoms of amino acid residues in the secondary structural elements is less than 2.0Å.

ALIPHATIC	Non-polar	G A P
		I L V
	Polar - uncharged	C S T M
		N Q
	Polar - charged	D E
		K R
AROMATIC		H F W Y

Abbreviations for amino acid residues are the standard 3-letter and/or 1-letter codes used in the art to refer to one of the 20 common L-amino acids.

SECONDARY STRUCTURE

The AR-LBD of the present invention is arranged in an α-helical sandwich. The AR-LBD comprises preferably eleven α-helices (H1, H3, H4, H5, H6, H7, H8, H9, H10, H11, H12). There is no H2 helix. Because both helices H4 and H5 and helices H11 and H12 are contiguous helices, the α-helical sandwich is regarded as comprising 9 α-helices and not 11 α-helices. The α- helices designated by the letter H in Figure 1. The helix number (such as H1) is indicated in black above the relevant helical sequence. The α-helical sandwich fold may further comprise preferably 3_{10} helices and preferably four short β strands (S1, S2, S3 and S4) associated in two anti-parallel β-sheets. The β strands are indicated by the letter E in Figure 1. The strand number (such as S1) is indicated in black above the relevant β sheet.

ALPHA HELIX (α-Helix)

As used herein, the term "α-helix" means a helical or spiral configuration of a polypeptide chain in which successive turns of the helix are held together by hydrogen bonds between the amide (peptide) links, the carbonyl group of any given residue being hydrogen-bonded to the imino group of the third residue

behind it in the chain. This is the case for all of the carbonyl and amide groups of the peptide bonds of the main chain. Typically, the α-helix has 3, 6 residues per turn and the translation or pitch along the helical axis is 1.5Å per residue and 5.4Å per turn. The helix may be left- or right-handed, the latter being much more common. The α-helix is one of the two basic elements of the secondary structure adopted by the polypeptide chain within the hydrophobic core of a globular protein. The other basic element is the β strand.

The AR-LBD of the present invention comprises a helix in the region of helix H6 which is an α-helix.

The AR-LBD of the present invention comprises contiguous helices. In this respect, helices H4 and H5 and helices H10 and H11 are contiguous. In contrast only the H10 and H11 sequences of the progesterone receptor were found to be contiguous (see Williams 1998).

CONTIGUOUS

As used herein, the term "contiguous helices" means helices which are connected to each other such as connected in line with each other.

BETA SHEET (β-SHEET) and BETA STRANDS (β STRANDS)

As used herein, the term "beta sheet (β-sheet) structure means a combination of several regions of a polypeptide chain. In contrast, the α helix, is built up from one continuous region. These regions, β strands, are usually from 5 to 10 residues long and are in an almost fully extended conformation with ϕ, ψ angles within the broad structurally allowed region in the upper left quadrant of the Ramachandran plot. These β strands are aligned adjacent to each other such that hydrogen bonds can form between C'O groups of one β strand and NH groups on

an adjacent β strand and vice versa. The β sheets that are formed from several such β strands are "pleated" with C_α atoms successively a little above and below the plane of the β sheet. The side chains follow this pattern such that within a β strand they also point alternatively above and below the β sheet.

PARALLEL AND ANTI-PARALLEL β-SHEETS

β strands can interact in two ways to form a pleated sheet. Either the amino acids in the aligned β strands can all run in the same biochemical direction, amino terminal to carboxy terminal, in which case the sheet is described as parallel, or the amino acids in successive strands can have alternating directions, amino terminal to carboxy terminal followed by carboxy terminal to amino terminal, followed by amino terminal to carboxy terminal, and so on, in which case the sheet is called antiparallel. Each of the two forms has a distinctive pattern of hydrogen bonding. The antiparallel β sheet has narrowly spaced hydrogen bond pairs that alternate with widely spaced pairs. Parallel β sheets have evenly spaced hydrogen bonds that angle across between the β strands. Within both types of β sheets all possible main chain hydrogen bonds are formed, except for the two flanking strands of the β sheet that only have one neighboring β strand.

The AR-LBD of the present invention comprises beta strands (β strands), designated by the letter E, which are make up sheets. These strands (S1, S2, S3 and S4) are arranged in the order in which they appear in the secondary structure as set out in Figure 1. These strands are arranged in two β-sheets.

KEY RESIDUES

As used herein the term "key residues" refers to one or more amino acid residues in an AR-LBD, capable of modulating ligand binding. The residues may be any one of the key residues within the AR-LBD as described herein or mutants

thereof or they may be residues with homology to the residues or mutants thereof. The key amino acid residues of the AR-LBD may be any one or more of the amino acid residues selected from the group consisting of: L701; L704; N705; L707; Q711; M742; L744; M745; M749; R752; F764; Q783; M787; F876; T877; L880; F891; M895 or a homologue or mutant thereof.

CONFORMATIONALLY CONSTRAINED RESIDUES

Preferably binding of the ligand to the AR-LBD causes conformational changes to the AR-LBD thereby inhibiting further binding thereto.
Preferably the ligand produced in accordance with the invention fills at least the LBP of the AR without perturbing the remainder of the AR structure.

Preferably the ligand interacts with conformationally constrained residue of the AR-LBD.
As used herein, the term "conformationally constrained residue" refers to a residue, such as an amino acid residue whose binding properties may be modulated through a mutation in that residue. The mutation in the amino acid residue may result in a change in the conformation of that residue. In particular, the mutation may result in a restricted/constrained conformation which may affect the interaction of a ligand with the hAR-LBD.

BINDING AFFINITY

Preferably the ligands of the present invention bind more effectively to the AR-LBD than androgen.

Preferably the ligands of the present invention bind with twice the binding affinity of androgen.

Preferably the ligands of the present invention bind with three times the affinity of androgen.

Preferably the ligands of the present invention bind with ten or more times the affinity of androgen.

Preferably the improvements in the interaction of a ligand with the AR-LBD are manifested as increases in binding affinity but may also include increases in receptor selectivity and/or modulation of efficacy.

Preferably the ligand inhibits the action of androgen and androgen mimetics by binding tightly to the AR-LBD but by not up-regulating androgen receptor gene expression.

MODEL

One aspect of the present invention is related to a model.

The crystal structure of the present invention can be used to generate a structural model such as a three dimensional (3D) structural model (or a representation thereof) comprising an AR-LBD or portion thereof. Alternatively, the crystal structure may be used to generate a computer model for the structure.

Preferably the crystal model comprising the AR-LBD is built from all or part of the X-ray diffraction data presented in Table 1 and/or the refinement statistics presented in Table 2.

Preferably the crystal model comprising the AR-LBD is built from all or part of the crystal co-ordinate data as shown in Table 4 (see Figure 6).

Thus, for example, the structural co-ordinates provided in the crystal.structure and/or model structure may comprise the amino acid residues of the AR-LBD, or

a portion of the AR-LBD or a homologue thereof useful in the modelling and design of test compounds capable of binding to the AR-LBD.

As used herein, the term "modelling" includes the quantitative and qualitative analysis of molecular structure and/or function based on atomic structural information and interaction models. The term "modelling" includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and other structure-based constraint models.

In another aspect of the present invention, the structural coordinates comprising the AR-LBD or a portion thereof may be applied to a model screening system.

As used herein, the term "model screening system" may be a solid 3D screening system or a computational screening system. Using this model, Test compounds can be modelled that fit spatially and preferentially into the AR-LBD.

In one preferred aspect, the test compounds are positioned in the AR-IBD through computational docking.

In another preferred aspect, the test compounds are positioned in the AR-BD through manual docking.

As used herein, the term "fits spatially" means that the three-dimensional structure of a ligand is accommodated geometrically in a cavity or pocket of an AR-IBD.

Preferably, modelling is performed using a computer and may be further optimized using known methods. This is called modelling optimisation. Overlays and super positioning with a three dimensional model of the AR-LBD, and/or a portion thereof, can also be used for modelling optimisation.

Alignment and/or modelling can be used as a guide for the placement of mutations on the AR-LBD surface to characterise the nature of the site in the context of a cell.

The structure coordinates of an AR-LBD structure described herein can be used as a model for determining the secondary or three-dimensional structures of additional native or mutated AR-LBD with unknown structure, as well as the structures of co-crystals of AR-LBD with compounds such as substrates and modulators (e.g. stimulators or inhibitors). The structure coordinates and models of an AR-LBD structure can also be used to determine solution-based structures of native or mutant AR-LBD.

Secondary or three-dimensional structure may be determined by applying the structural coordinates of an AR-LBD structure to other data such as an amino acid sequence, X-ray crystallographic diffraction data, or nuclear magnetic resonance (NMR) data. Homology modeling, molecular replacement, and nuclear magnetic resonance methods using these other data sets are described below.

Homology modeling (also known as comparative modeling or knowledge-based modeling) methods develop a three dimensional model from a polypeptide sequence based on the structures of known proteins (e.g. native or mutated AR-LBD). In the present invention the method utilizes a computer representation of an AR-LBD structure or a complex of same, a computer representation of the amino acid sequence of a polypeptide with an unknown structure (additional native or mutated AR-LBD), and standard computer representations of the structures of amino acids. The method in particular comprises the steps of; (a) identifying structurally conserved and variable regions in the known structure; (b) aligning the amino acid sequences of the known structure and unknown structure (c) generating coordinates of main chain atoms and side chain atoms in structurally conserved and variable regions of the unknown structure based on the

coordinates of the known structure thereby obtaining a homology model; and (d) refining the homology model to obtain a three dimensional structure for the unknown structure. This method is well known to those skilled in the art (Greer, 1985, Science 228, 1055; Bundell et al 1988, Eur. J. Biochem. 172, 513; Knighton et al., 1992, Science 258:130-135, http://biochem.vt.edu/courses/modeling/homology.htn). Computer programs that can be used in homology modeling are Quanta and the Homology module in the Insight II modeling package distributed by Molecular Simulations Inc, or MODELLER (Rockefeller University, www.iucr.ac.uk/sinris-top/logical/prg-modeller.html).

In step (a) of the homology modeling method, the known AR-LBD structure is examined to identify the structurally conserved regions (SCRs) from which an average structure, or framework, can be constructed for these regions of the protein. Variable regions (VRs), in which known structures may differ in conformation, also must be identified. SCRs generally correspond to the elements of secondary structure, such as alpha-helices and beta-sheets, and to ligand- and substrate-binding sites (e.g. acceptor and donor binding sites). The VRs usually lie on the surface of the proteins and form the loops where the main chain turns.

Many methods are available for sequence alignment of known structures and unknown structures. Sequence alignments generally are based on the dynamic programming algorithm of Needleman and Wunsch [J. Mol. Biol. 48: 442-453, 1970]. Current methods include FASTA, Smith-Waterman, and BLASTP, with the BLASTP method differing from the other two in not allowing gaps. Scoring of alignments typically involves construction of a 20x20 matrix in which identical amino acids and those of similar character (i.e., conservative substitutions) may be scored higher than those of different character. Substitution schemes which may be used to score alignments include the scoring matrices PAM (Dayhoff et al., Meth. Enzymol. 91: 524-545, 1983), and BLOSUM (Henikoff and Henikoff, Proc. Nat. Acad. Sci. USA 89: 10915-`0919,

1992), and the matrices based on alignments derived from three-dimensional structures including that of Johnson and Overington (JO matrices) (J. Mol. Biol. 233: 716-738, 1993).

Alignment based solely on sequence may be used; however, other structural features also may be taken into account. In Quanta, multiple sequence alignment algorithms are available that may be used when aligning a sequence of the unknown with the known structures. Four scoring systems (i.e. sequence homology, secondary structure homology, residue accessibility homology, CA-CA distance homology) are available, each of which may be evaluated during an alignment so that relative statistical weights may be assigned.

When generating coordinates for the unknown structure, main chain atoms and side chain atoms, both in SCRs and VRs need to be modeled. A variety of approaches known to those skilled in the art may be used to assign coordinates to the unknown. In particular, the coordinates of the main chain atoms of SCRs will be transferred to the unknown structure. VRs correspond most often to the loops on the surface of the polypeptide and if a loop in the known structure is a good model for the unknown, then the main chain coordinates of the known structure may be copied. Side chain coordinates of SCRs and VRs are copied if the residue type in the unknown is identical to or very similar to that in the known structure. For other side chain coordinates, a side chain rotamer library may be used to define the side chain coordinates. When a good model for a loop cannot be found fragment databases may be searched for loops in other proteins that may provide a suitable model for the unknown. If desired, the loop may then be subjected to conformational searching to identify low energy conformers if desired.

Once a homology model has been generated it is analyzed to determine its correctness. A computer program available to assist in this analysis is the Protein Health module in Quanta which provides a variety of tests. Other programs that provide structure analysis along with output include PROCHECK and 3D-

Profiler [Luthy R. et al, Nature 356: 83-85, 1992; and Bowie, J.U. et al, Science 253: 164-170, 1991]. Once any irregularities have been resolved, the entire structure may be further refined. Refinement may consist of energy minimization with restraints, especially for the SCRs. Restraints may be gradually removed for subsequent minimizations. Molecular dynamics may also be applied in conjunction with energy minimization.

Using the structure coordinates of the crystal complexes provided by this invention, molecular replacement may be used to determine the structure coordinates of a crystalline mutant or homologue of AR-LBD or of a related protein.

Molecular replacement involves applying a known structure to solve the X-ray crystallographic data set of a polypeptide of unknown structure (e.g. native or mutated AR-LBD). The method can be used to define the phases describing the X-ray diffraction data of a polypeptide of unknown structure when only the amplitudes are known. Commonly used computer software packages for molecular replacement are X-PLOR (Brunger 1992, Nature 355: 472-475), AMoRE (Navaza, 1994, Acta Crystallogr. A50:157-163), the CCP4 package (Collaborative Computational Project, Number 4, "The CCP4 Suite: Programs for Protein Crystallography", Acta Cryst., Vol. D50, pp. 760-763, 1994), and the MERLOT package (P.M.D. Fitzgerald, J. Appl. Cryst., Vol. 21, pp. 273-278, 1988). It is preferable that the resulting structure not exhibit a root-mean-square deviation of more than 3 Å.

Molecular replacement computer programs generally involve the following steps: (1) determining the number of molecules in the unit cell and defining the angles between them (self rotation function); (2) rotating the known structure (e.g. AR-LBD) against diffraction data to define the orientation of the molecules in the unit cell (rotation function); (3) translating the known structure in three dimensions to correctly position the molecules in the unit cell (translation function); (4)

determining the phases of the X-ray diffraction data and calculating an R-factor calculated from the reference data set and from the new data wherein an R-factor between 30-50% indicates that the orientations of the atoms in the unit cell have been reasonably determined by the method; and (5) optionally, decreasing the R-factor to about 20% by refining the new electron density map using iterative refinement techniques known to those skilled in the art (refinement).

In an embodiment of the invention, a method is provided for determining three dimensional structures of polypeptides with unknown structure (e.g. additional native or mutated AR-LBD) by applying the structural coordinates of an AR-LBD structure to provide an X-ray crystallographic data set for a polypeptide of unknown structure, and (b) determining a low energy conformation of the resulting structure.

The structural coordinates of an AR-LBD structure may be applied to nuclear magnetic resonance (NMR) data to determine the three dimensional structures of polypeptides (e.g. additional native or mutated AR-LBD). (See for example, Wuthrich, 1986, John Wiley and Sons, New York: 176-199; Pflugrath et al., 1986, J. Molecular Biology 189: 383-386; Kline et al., 1986 J. Molecular Biology 189:377-382). While the secondary structure of a polypeptide may often be determined by NMR data, the spatial connections between individual pieces of secondary structure are not as readily determined. The structural coordinates of a polypeptide defined by X-ray crystallography can guide the NMR spectroscopist to an understanding of the spatial interactions between secondary structural elements in a polypeptide of related structure. Information on spatial interactions between secondary structural elements can greatly simplify Nuclear Overhauser Effect (NOE) data from two-dimensional NMR experiments. In addition, applying the structural coordinates after the determination of secondary structure by NMR techniques simplifies the assignment of NOE's relating to particular amino acids in the polypeptide sequence and does not greatly bias the NMR analysis of polypeptide structure.

This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal. Lattman, E., "Use of the Rotation and Translation Functions", in Methods in Enzymology, 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York, (1972).

Other molecular modelling techniques may also be employed in accordance with this invention. See, e.g., Cohen, N. C. *et al*, "Molecular Modelling Software and Methods for Medicinal Chemistry", J. Med. Chem., 33, pp. 883-894 (1990). See also, Navia, M. A. and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

The present invention also relates to a method of screening for a ligand capable of binding to the AR-LBD and/or which are capable of modulating the binding capacity of the AR-LBD wherein said method comprises the use of the crystal or model according to the invention.

The method may employ a solid 3D screening system or a computational screening system. Using these systems, test compounds may be screened to find those which interact spatially and preferentially with the AR-LBD, through either computational or manual docking.

TEST COMPOUNDS

In one aspect, the invention relates to a method of screening for a ligand capable of binding to an AR-LBD, wherein the AR-LBD is defined by the amino acid residue structural coordinates given above, the method comprising contacting the AR-LBD with a test compound and determining if said test compound binds to said AR-LBD.

As used herein, the term "test compound" includes, but is not limited to, a compound which may be obtainable from or produced by any suitable source, whether natural or not. The test compound may be designed or obtained from a library of compounds which may comprise peptides, as well as other compounds, such as small organic molecules and particularly new lead compounds. By way of example, the test compound may be a natural substance, a biological macromolecule, or an extract made from biological materials such as bacteria, fungi, or animal (particularly mammalian) cells or tissues, an organic or an inorganic molecule, a synthetic test compound, a semi-synthetic test compound, a structural or functional mimetic, a peptide, a peptidomimetics, a derivatised test compound, a peptide cleaved from a whole protein, or a peptides synthesised synthetically (such as, by way of example, either using a peptide synthesizer or by recombinant techniques or combinations thereof, a recombinant test compound, a natural or a non-natural test compound, a fusion protein or equivalent thereof and mutants, derivatives or combinations thereof.

MODULATING

The term "modulating" means inducing an increase or a decrease in the activity of the androgen receptor through binding of a test compound to an AR-LBD. The term also encompasses removal of the activity of the receptor.

MIMETIC

As used herein, the term "mimetic" relates to any chemical which includes, but is not limited to, a peptide, polypeptide, antibody or other organic chemical which has the same qualitative activity or effect as a known test compound. That is, the mimetic is a functional equivalent of a known test compound (such as a known ligand capable of binding to the AR-LBD).

DERIVATIVE

The term "derivative" or "derivatised" as used herein includes chemical modification of a test compound. Illustrative of such chemical modifications would be replacement of hydrogen by a halo group, an alkyl group, an acyl group or an amino group.

Typically the test compound will be prepared by recombinant DNA techniques and/or chemical synthesis techniques.

Once a test compound capable of interacting with a key amino acid residue in the AR-LBD has been identified, further steps may be carried out either to select and/or to modify compounds and/or to modify existing compounds, to modulate the interaction with the key amino acid residues in the AR-LBD.

BIOLOGICAL SCREENS

Test compounds and ligands which are identified with the crystal of the present invention can be screened in assays such as are well known in the art. Screening can be, for example *in vitro*, in cell culture, and/or *in vivo*. Biological screening assays preferably center on activity-based response models, binding assays (which measure how well a compound binds to the receptor), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity-high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity. The biological assay, may also be an assay for ligand binding activity a compound that selectively binds to the LBD compared to other nuclear receptors.

In one embodiment, the present invention provides a method of screening for a test compound capable of interacting with a key amino acid residue of the AR-LBD .

Another preferred aspect of the invention provides a process comprising the steps of:

(a) performing the method of screening for a ligand as described above;

(b) identifying one or more ligands capable of binding to a ligand binding domain; and

(c) preparing a quantity of said one or more ligands.

A further preferred aspect of the invention provides a process comprising the steps of:

(a) performing the method of screening for a ligand as described above;

(b) identifying one or more ligands capable of binding to an AR-LBD; and

(c) preparing a pharmaceutical composition comprising said one or more ligands.

Yet another preferred aspect of the invention provides a process comprising the steps of:

(a) performing the method of screening for a ligand as described above;

(b) identifying one or more ligands capable of binding to an AR-LBD;

(c) modifying said one or more ligands capable of binding to an AR-LBD;

(d) performing said method of screening for a ligand as described above;

(e) optionally preparing a pharmaceutical composition comprising said one or more ligands.

Thus, the structural information from the crystal structure of the present invention is useful in the design of potential ligands capable of interacting with the AR-LBD and/or capable of modulating the DNA binding capacity of the AR-LBD, and

the models of the present invention are useful to examine the effect such a ligand is likely to have on the structure and/or function of the AR-LBD.

In one aspect the present invention relates to a ligand identified using such screening methods.

LIGAND

As used herein, the term "ligand" refers to a test compound capable of binding to one or more key residues in the LBD. Such a ligand may also be referred to as an androgen receptor binding compound. Preferably the ligand is capable of modulating the activity of AR-LBD.

IDENTIFICATION OF MODULATORS OF AR-LBD

Modulators (e.g. inhibitors) of a AR-LBD may be designed and identified that may modify a AR-LBD involved in a clinical disorder. The rational design and identification of modulators of AR-LBD can be accomplished by utilizing the atomic structural coordinates that define an AR-LBD structure, or a part thereof. Structure-based modulator design identification methods are powerful techniques that can involve searches of computer data bases containing a variety of potential modulators and chemical functional groups. (See Kuntz et al., 1994, Acc. Chem. Res. 27:117; Guida, 1994, Current Opinion in Struc. Biol. 4: 777; and Colman, 1994, Current Opinion in Struc. Biol. 4: 868, for reviews of structure-based drug design and identification;and Kuntz et al 1982, J. Mol. Biol. 162:269; Kuntz et al., 1994, Acc. Chem. Res. 27: 117; Meng et al., 1992, J. Compt. Chem. 13: 505; Bohm, 1994, J. Comp. Aided Molec. Design 8: 623 for methods of structure-based modulator design).

The AR-LBD structures, and parts thereof described herein, and the structures of other polypeptides determined by the homology modeling, molecular

replacement, and NMR techniques described herein can also be applied to modulator design and identification methods.

Modulators of AR-LBD may be identified by docking the computer representation of compounds from a data base of molecules. Data bases which may be used include ACD (Molecular Designs Limited), NCI (National Cancer Institute), CCDC (Cambridge Crystallographic Data Center), CAST (Chemical Abstract Service), Derwent (Derwent Information Limited), Maybridge (Maybridge Chemical Company Ltd), Aldrich (Aldrich Chemical Company), DOCK (University of California in San Francisco), and the Directory of Natural Products (Chapman & Hall). Computer programs such as CONCORD (Tripos Associates) or DB-Converter (Molecular Simulations Limited) can be used to convert a data set represented in two dimensions to one represented in three dimensions.

The computer programs may comprise the following steps:

(a) docking a computer representation of a structure of a compound into a computer representation of an AR-LBD defined in accordance with the invention using the computer program, or by interactively moving the representation of the compound into the representation of the binding site;

(b) characterizing the geometry and the complementary interactions formed between the atoms of the binding site and the compound; optionally

(c) searching libraries for molecular fragments which can fit into the empty space between the compound and binding site and can be linked to the compound; and

(d) linking the fragments found in (c) to the compound and evaluating the new modified compound.

Methods are also provided for identifying a potential modulator of an AR-LBD function by docking a computer representation of a compound with a computer representation of a structure of an AR-LBD that is defined by atomic interactions,

atomic contacts, or atomic structural coordinates described herein. In an embodiment the method comprises the following steps:

(a) docking a computer representation of a compound from a computer data base with a computer representation of a selected site (e.g. the inhibitor binding site) on a AR-LBD structure defined in accordance with the invention to obtain a complex;

(b) determining a conformation of the complex with a favourable geometric fit and favourable complementary interactions; and

(c) identifying compounds that best fit the selected site as potential modulators of the AR-LBD.

"Docking" refers to a process of placing a compound in close proximity with an active site of a polypeptide (i.e. an AR-LBD), or a process of finding low energy conformations of a compound/polypeptide complex (i.e. compound/AR-LBD complex).

Examples of other computer programs that may be used for structure-based modulator design are CAVEAT (Bartlett et al., 1989, in "Chemical and Biological Problems in Molecular Recognition", Roberts, S.M. Ley, S.V.; Campbell, N.M. eds; Royal Society of Chemistry: Cambridge, pp 182-196); FLOG (Miller et al., 1994, J. Comp. Aided Molec. Design 8:153); PRO Modulator (Clark et al., 1995 J. Comp. Aided Molec. Design 9:13); MCSS (Miranker and Karplus, 1991, Proteins: Structure, Fuction, and Genetics 8:195); and, GRID (Goodford, 1985, J. Med. Chem. 28:849).

In an embodiment of the invention, a method is provided for identifying potential modulators of AR-LBD function. The method utilizes the structural coordinates of an AR-LBD three dimensional structure, or binding site thereof. The method comprises the steps of (a) generating a computer representation of an AR-LBD structure, and docking a computer representation of a compound from a computer data base with a computer representation of the AR-LBD to form a complex; (b)

determining a conformation of the complex with a favourable geometric fit or favorable complementary interactions; and (c) identifying compounds that best fit the AR-LBD as potential modulators of AR-LBD function. The initial AR-LBD structure may or may not have compounds bound to it. A favourable geometric fit occurs when the surface areas of a compound in a compound-AR-LBD complex is in close proximity with the surface area of the AR-LBD without forming unfavorable interactions. A favourable complementary interaction occurs where a compound in a compound-AR-LBD complex interacts by hydrophobic, aromatic, ionic, or hydrogen donating and accepting forces, with the AR-LBD without forming unfavorable interactions. Unfavourable interactions may be steric hindrance between atoms in the compound and atoms in the AR-LBD.

In another embodiment, potential modulators are identified utilizing an AR-LBD structure with or without compounds bound to it. The method comprises the steps of (a) modifying a computer representation of an AR-LBD having one or more compounds bound to it, where the computer representations of the compound or compounds and AR-LBD are defined by atomic structural coordinates; (b) determining a conformation of the complex with a favorable geometric fit and favorable complementary interactions; and (c) identifying the compounds that best fit the AR-LBD as potential modulators. A computer representation may be modified by deleting or adding a chemical group or groups. Computer representations of the chemical groups can be selected from a computer database.

Another way of identifying potential modulators is to modify an existing modulator in a polypeptide binding site. The computer representation of modulators can be modified within the computer representation of an AR-LBD. This technique is described in detail in Molecular Simulations User Manual, 1995 in LUDI. The computer representation of a modulator may be modified by deleting a chemical group or groups, or by adding a chemical group or groups. After each modification to a compound, the atoms of the modified compound and binding site can be shifted in conformation and the distance between the

modulator and the binding site atoms may be scored on the basis of geometric fit and favourable complementary interactions between the molecules. Compounds with favourable scores are potential modulators.

Compounds designed by modulator building or modulator searching computer programs may be screened to identify potential modulators. Examples of such computer programs include programs in the Molecular Simulations Package (Catalyst), ISIS/HOST, ISIS/BASE, and ISIS/DRAW (Molecular Designs Limited), and UNITY (Tripos Associates). A building program may be used to replace computer representations of chemical groups in a compound complexed with an AR-LBD with groups from a computer database. A searching program may be used to search computer representations of compounds from a computer database that have similar three dimensional structures and similar chemical groups as a compound that binds to an AR-LBD. The programs may be operated on the structure of the AR-LBD structure.

A typical program may comprise the following steps:

(a) mapping chemical features of a compound such as by hydrogen bond donors or acceptors, hydrophobic/lipophilic sites, positively ionizable sites, or negatively ionizable sites;

(b) adding geometric constraints to selected mapped features;

(c) searching data bases with the model generated in (b).

In an embodiment of the invention a method of identifying potential modulators of an AR-LBD is provided using the three dimensional conformation of the AR-LBD in various modulator construction or modulator searching computer programs on compounds complexed with the AR-LBD. The method comprises the steps of (a) generating a computer representation of one or more compounds complexed with an AR-LBD; (b) (i) searching a data base for a compound with a similar geometric structure or similar chemical groups to the generated compounds using a computer program that searches computer representations of

compounds from a database that have similar three dimensional structures and similar chemical groups, or (ii) replacing portions of the compounds complexed with the AR-LBD with similar chemical structures (i.e. nearly identical shape and volume) from a database using a compound construction computer program that replaces computer representations of chemical groups with groups from a computer database, where the representations of the compounds are defined by structural coordinates.

A compound that interacts with an AR-LBD identified using a method of the invention may be used as a modulator of any AR-LBD or composition bearing the interacting binding domain. Therefore, the invention features a modulator of an AR-LBD identified by a method of the invention.

The invention further contemplates a method for designing potential inhibitors of an AR-LBD comprising the step of using the structural coordinates of an inhibitor or substrate or parts thereof, defined in relation to its spatial association with an AR-LBD structure to generate a compound that is capable of associating with the AR-LBD.

In an embodiment of the invention, a method is provided for designing potential inhibitors of an AR-LBD comprising the step of using the structural coordinates of AR-LBD in Table 4 to generate a compound for associating with the active site of an AR-LBD. The following steps are employed in a particular method of the invention: (a) generating a computer representation of AR-LBD defined by its structural coordinates listed in Table 4; (b) searching for molecules in a data base that are structurally or chemically similar to the defined AR-LBD, using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

It will be appreciated that a modulator of an AR-LBD may be identified by generating an actual three-dimensional model of a binding cavity, synthesizing a compound, and examining the components to find whether the required interaction occurs.

Potential modulators of AR-LBD identified using the above-described methods may be prepared using methods described in standard reference sources utilized by those skilled in the art. For example, organic compounds may be prepared by organic synthetic methods described in references such as March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, New York, McGraw Hill.

The invention also relates to a potential modulator identified by the methods of the invention. In particular, classes of modulators of AR-LBD are provided that are based on the three-dimensional structure of an inhibitor's or modulator's spatial association with an AR-LBD structure.

The invention contemplates all optical isomers and racemic forms of the modulators of the invention.

"Modulator" refers to a molecule which changes or alters the biological activity of a AR-LBD. A modulator may increase or decrease AR-LBD activity, or change its characteristics, or functional or immunological properties. It may be an inhibitor that decreases the biological or immunological activity of the protein. A modulator may enhance or inhibit a biological activity of AR-LBD.

Modulators include but are not limited to peptides, members of random peptide libraries and combinatorial chemistry-derived molecular libraries, phosphopeptides (including members of random or partially degenerate, directed phosphopeptide libraries), antibodies, carbohydrates, nucleosides or nucleotides

or parts thereof, and small organic or inorganic molecules. A modulator may be an endogenous physiological compound, or it may be a natural or synthetic compound.

LIGAND

The term "ligand" includes, but is not limited to, steroidal and non-steroidal ligands. The ligands may be natural or synthetic. The ligands may be structurally novel AR-LBD ligands. Alternatively, the ligands may be analogues of known AR-LBD ligands but with improved properties. The ligand may be an androgen mimetic. The ligand may be capable of modulating (e.g. upregulating) androgen receptor gene expression. Alternatively, the ligand may be capable of blocking the activity of androgens by binding to an AR-LBD with a high affinity. The ligand may be capable of down regulating androgen receptor gene expression. The term "ligand" also refers to a chemically modified ligand.

The ligand may act, for example, as an agonist, a partial agonist, an antagonist, and/or a competitive antagonist of the androgen receptor.

For some embodiments, the ligand is in a purified and/or isolated form.

DESIGNER LIGANDS

As used herein, the term means "designer ligands" refers to test compounds which are likely to bind to the AR-LBD based on their three dimensional shape compared to that of the androgen receptor and in particular the AR-LBD.

Preferably, those compounds have a structure which is complementary to that of the AR-
LBD.

Preferably the ligands comprise ligand substituents which compensate for the structural changes in the ligand binding pocket (LBP) between the wild type and mutant AR-LBDs.

The test compound may be tested for its interaction with an interacting amino acid residue in the AR-LBD. Alternatively, the test compound may affect ligand binding by acting either as an agonists or an antagonists.

AGONIST

As used herein, the term "agonist" means any ligand, which is capable of binding to an AR-LBD and which is capable of increasing a proportion of the AR that is in an active form, resulting in an increased biological response. The term includes partial agonists and inverse agonists.

PARTIAL AGONIST

As used herein, the term "partial agonist" means an agonist that is unable to evoke the maximal response of a biological system, even at a concentration sufficient to saturate the specific receptors.

INVERSE AGONIST

As used herein, the term "partial inverse agonist" is an inverse agonist that evokes a submaximal response to a biological system, even at a concentration sufficient to saturate the specific receptors. At high concentrations, it will diminish the actions of a full inverse agonist.

ANTAGONIST

As used herein, the term "antagonist" means any agent that reduces the action of another agent, such as an agonist. The antagonist may act at the same receptor as the agonist. The antagonistic action may result from a combination of the substance being antagonised (chemical antagonism) or the production of an opposite effect through a different receptor (functional antagonism or physiological antagonism) or as a consequence of competition for the binding site of an intermediate that links receptor activation to the effect observed (indirect antagonism).

COMPETITIVE ANTAGONIST

As used herein, the term "competitive antagonism" refers to the competition between an agonist and an antagonist for a receptor that occurs when the binding of agonist and antagonist becomes mutually exclusive. This may be because the agonist and antagonist compete for the same binding site or combine with adjacent but overlapping sites. A third possibility is that different sites are involved but that they influence the receptor macromolecules in such a way that agonist and antagonist molecules cannot be bound at the same time. If the agonist and antagonist form only short lived combinations with the receptor so that equilibrium between agonist, antagonist and receptor is reached during the presence of the agonist, the antagonism will be surmountable over a wide range of concentrations. In contrast, some antagonists, when in close enough proximity to their binding site, may form a stable covalent bond with it and the antagonism becomes insurmountable when no spare receptors remain.

In one aspect, the identified ligand may act as a ligand model (for example, a template) for the development of other compounds.

LIGAND MODEL

The term "ligand model" refers to the structural coordinates of a compound that fits into the AR-ligand binding domain (LBD) and which may be used for modeling to identify and/or design ligands (designer ligands) capable of binding to the AR-LBD, such as for the subsequent modulation thereof.

One skilled in the art may use one of several methods to test compounds for their ability to associate with AR-LBD. This process may begin by visual inspection of, for example, a target site on the computer screen based on the structure coordinates given in Table 4. Selected test compounds may then be positioned in a variety of orientations, or docked, within an individual target site of AR-LBD as defined supra. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.
Specialized computer programs may also assist in the process of selecting potential ligands. These include:

1. GRID (Goodford, P. J., "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", J. Med. Chem., 28, pp. 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.

2. MCSS (Miranker, A. and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure. Function and Genetics, 11, pp. 29-34 (1991)). MCSS is available from Molecular Simulations, Burlington, Mass.

3. AUTODOCK (Goodsell, D. S. and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins: Structure. Function, and Genetics, 8, pp. 195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, Calif.

4. DOCK (Kuntz, I. D. et al., "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., 161, pp. 269-288 (1982)). DOCK is available from University of California, San Francisco, Calif.

Once a ligand has been optimally selected or designed, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit to AR-LBD by the same computer methods described above.

Preferably, positions for substitution are selected based on the predicted binding orientation of a test compound to the AR-LBD.

The ligands of the present invention may be natural or synthetic. The term "ligand" also refers to a chemically modified ligand.

SYNTHESIS METHODS

The ligand of the present invention or mimetics thereof may be produced using chemical methods to synthesize the ligand in whole or in part. For example, peptides can be synthesized by solid phase techniques, cleaved from the resin, and purified by preparative high performance liquid chromatography (e.g., Creighton (1983) Proteins Structures And Molecular Principles, WH Freeman and Co, New York NY). The composition of the synthetic peptides may be confirmed by amino acid analysis or sequencing (e.g., the Edman degradation procedure; Creighton, *supra*).

Direct synthesis of the ligand or mimetics thereof can be performed using various solid-phase techniques (Roberge JY *et al* (1995) Science 269: 202-204) and automated synthesis may be achieved, for example, using the ABI 43 1 A Peptide Synthesizer (Perkin Elmer) in accordance with the instructions provided by the manufacturer. Additionally, the amino acid sequences obtainable from the ligand, or any part thereof, may be altered during direct synthesis and/or combined using chemical methods with a sequence from other subunits, or any part thereof, to produce a variant ligand.

In an alternative embodiment of the invention, the coding sequence of the ligand or mimetics thereof may be synthesized, in whole or in part, using chemical methods well known in the art (see Caruthers MH *et al* (1980) Nuc Acids Res Symp Ser 215-23, Horn T *et al* (1980) Nuc Acids Res Symp Ser 225-232).

Hence, the ligands may be chemically synthesised or they may be prepared using recombinant techniques.

In one aspect, preferably, the ligand is prepared by the use of chemical synthesis techniques.

RECOMBINANT METHODS

In another aspect, preferably the ligands of the present invention may be produced from host cells using recombinant techniques.

A wide variety of host cells can be employed for expression of the nucleotide sequences encoding the ligands of the present invention. These cells may be both prokaryotic and eukaryotic host cells. Suitable host cells include bacteria such as *E. coli*, yeast, filamentous fungi, insect cells, mammalian cells, typically immortalized, e.g., mouse, CHO, human and monkey cell lines and derivatives thereof. Preferred host cells are able to process the expression products to

produce an appropriate mature polypeptide. Processing includes but is not limited to glycosylation, ubiquitination, disulfide bond formation and general post-translational modification.

CHEMICAL MODIFICATION

In one embodiment of the present invention, the ligand may be a chemically modified ligand.

The chemical modification of a ligand and/or a key amino acid residue of the present invention may either enhance or reduce hydrogen bonding interaction, charge interaction, hydrophobic interaction, Van Der Waals interaction or dipole interaction between the ligand and the key amino acid residue(s) of the AR-LBD. By way of example, steric hinderance is a common means of changing the interaction of the AR-LBD binding domain with the activation domain.

Preferably such modifications involve the addition of substituents onto a test compound such that the substituents are positioned to collide or to bind preferentially with one or more amino acid residues that correspond to the key amino acid residues of AR-LBD of the present invention.

COMPARATIVE MODELS

The unique features involved in AR selective ligand binding can be identified by comparing crystal structures of different steroid receptors, such as the AR and the progesterone (PR) receptors and/or isoforms of the same type of receptor.

In a seventh aspect the present invention provides the use of a ligand identified by a method of screening which comprises the use of a crystal structure comprising an AR-LBD in the preparation of a medicament to prevent and/or treat androgen related disorders.

DISORDERS

The term androgen related disorders relates to disorder such as prostrate cancer (PC), androgen insensitivity syndrome (AIS), partial androgen insensitivity syndrome (PAIS), mild androgen insensitivity syndrome (MAIS) and complete androgen insensitivity syndrome (CAIS).

PHARMACEUTICAL COMPOSITIONS

In a further aspect, the present invention provides a pharmaceutical composition, which comprises a ligand according to the present invention and optionally a pharmaceutically acceptable carrier, diluent or excipient (including combinations thereof). The pharmaceutical composition may comprise or may be used in conjunction with an additional pharmaceutically active compound or composition.

The pharmaceutical compositions may be for human or animal usage in human and veterinary medicine and will typically comprise any one or more of a pharmaceutically acceptable diluent, carrier, or excipient. Acceptable carriers or diluents for therapeutic use are well known in the pharmaceutical art, and are described, for example, in Remington's Pharmaceutical Sciences, Mack Publishing Co. (A. R. Gennaro edit. 1985). The choice of pharmaceutical carrier, excipient or diluent can be selected with regard to the intended route of administration and standard pharmaceutical practice. The pharmaceutical compositions may comprise as - or in addition to - the carrier, excipient or diluent any suitable binder(s), lubricant(s), suspending agent(s), coating agent(s), solubilising agent(s).

Preservatives, stabilizers, dyes and even flavouring agents may be provided in the pharmaceutical composition. Examples of preservatives include sodium

benzoate, sorbic acid and esters of p-hydroxybenzoic acid. Antioxidants and suspending agents may be also used.

There may be different composition/formulation requirements dependent on the different delivery systems. By way of example, the pharmaceutical composition of the present invention may be formulated to be delivered using a mini-pump or by a mucosal route, for example, as a nasal spray or aerosol for inhalation or ingestable solution, or parenterally in which the composition is formulated by an injectable form, for delivery, by, for example, an intravenous, intramuscular or subcutaneous route. Alternatively, the formulation may be designed to be delivered by both routes.

Where the pharmaceutical composition is to be delivered mucosally through the gastrointestinal mucosa, it should be able to remain stable during transit though the gastrointestinal tract; for example, it should be resistant to proteolytic degradation, stable at acid pH and resistant to the detergent effects of bile.

Where appropriate, the pharmaceutical compositions can be administered by inhalation, in the form of a suppository or pessary, topically in the form of a lotion, solution, cream, ointment or dusting powder, by use of a skin patch, orally in the form of tablets containing excipients such as starch or lactose or chalk, or in capsules or ovules either alone or in admixture with excipients, or in the form of elixirs, solutions or suspensions containing flavouring or colouring agents, or they can be injected parenterally, for example intravenously, intramuscularly or subcutaneously. For parenteral administration, the compositions may be best used in the form of a sterile aqueous solution which may contain other substances, for example enough salts or monosaccharides to make the solution isotonic with blood. For buccal or sublingual administration the compositions may be administered in the form of tablets or lozenges which can be formulated in a conventional manner.

ADMINISTRATION

The invention further provides a method of preventing and/or treating an androgen related disorder in a mammal, the method comprising administering to a mammal a ligand which binds to at least the AR-LBD with high affinity, and in some cases to such an extent so as to modulate said AR-LBD. In one aspect, the block binding of further ligands to at least the AR-LBD. Such ligands may be useful in, for example, the treatment of AR mediated disorders in males or females.

Typically, a physician will determine the actual dosage which will be most suitable for an individual subject and it will vary with the age, weight and response of the particular patient and severity of the condition. The dosages below are exemplary of the average case. There can, of course, be individual instances where higher or lower dosage ranges are merited.

The compositions (or component parts thereof) of the present invention may be administered orally. In addition or in the alternative the compositions (or component parts thereof) of the present invention may be administered by direct injection. In addition or in the alternative the compositions (or component parts thereof) of the present invention may be administered topically. In addition or in the alternative the compositions (or component parts thereof) of the present invention may be administered by inhalation. In addition or in the alternative the compositions (or component parts thereof) of the present invention may also be administered by one or more of: parenteral, mucosal, intramuscular, intravenous, subcutaneous, intraocular or transdermal administration means, and are formulated for such administration.

By way of further example, the pharmaceutical composition of the present invention may be administered in accordance with a regimen of 1 to 10 times per day, such as once or twice per day. The specific dose level and frequency of

dosage for any particular patient may be varied and will depend upon a variety of factors including the activity of the specific compound employed, the metabolic stability and length of action of that compound, the age, body weight, general health, sex, diet, mode and time of administration, rate of excretion, drug combination, the severity of the particular condition, and the host undergoing therapy.

The term "administered" also includes but is not limited to delivery by a mucosal route, for example, as a nasal spray or aerosol for inhalation or as an ingestable solution; a parenteral route where delivery is by an injectable form, such as, for example, an intravenous, intramuscular or subcutaneous route.

Hence, the pharmaceutical composition of the present invention may be administered by one or more of the following routes: oral administration, injection (such as direct injection), topical, inhalation, parenteral administration, mucosal administration, intramuscular administration, intravenous administration, subcutaneous administration, intraocular administration or transdermal administration.

STRUCTURAL STUDIES

One aspect of the invention provides to a method of determining the secondary and/or tertiary structures of polypeptides with unknown structures comprising the step of using a crystal structure or model of the invention.

The polypeptide under investigation is preferably structurally or functionally related to the androgen receptor ligand binding domain. For example, the polypeptide may show a degree of homology over some or all parts of the primary amino acid sequence.

As applied to polypeptides, the term "substantial sequence identity" means that two peptide sequences, when optimally aligned, such as by the programs GAP or BESTFIT using default gap, share at least 40%, 50%, 60%, 65%, 70%, 75%, 80%, or 85% sequence identity, preferably at least 90 percent sequence identity, more preferably at least 95 percent sequence identity or more. Preferably, residue positions which are not identical differ by conservative amino acid substitutions. For example, the substitution of amino acids having similar chemical properties such as charge or polarity are not likely to effect the properties of a protein. Examples include glutamine for asparagine or glutamic acid for aspartic acid.

In a further embodiment, the invention relates to a method of determining three dimensional structures of polypeptides with unknown structures, preferably a native or mutated AR-LBD by applying the structural coordinates of an AR-LBD structure of the invention to nuclear magnetic resonance (NMR) data of the unknown structure. This method comprises the steps of: (a) determining the secondary structure of an unknown structure using NMR data; and (b) simplifying the assignment of through-space interactions of amino acids. The term " through-space interactions" defines the orientation of the secondary structural elements in the three dimensional structure and the distances between amino acids from different portions of the amino acid sequence. The term "assignment" defines a method of analyzing NMR data and identifying which amino acids give rise to signals in the NMR spectrum.

The polypeptide may, for example be a mutant form of an AR-LBD. The term "mutant" refers to a polypeptide that is obtained by replacing at least one amino acid residue in a native AR-LBD with a different amino acid residue. Mutation can also be accomplished by adding and/or deleting amino acid residues within the native AR-LBD or part thereof. A mutant may or may not be functional.

Alternatively, the polypeptide may be an AR-LBD from a different species.

Alternatively, the polypeptide may perform an analogous function or be suspected to show a similar binding mechanism to the AR-LBD.

ANDROGEN RECEPTOR LIGAND BINDING DOMAIN STRUCTURES

The present invention provides a secondary or three-dimensional structure of an AR-LBD or part thereof. In an embodiment the structure is a crystalline form An AR-LBD structure may comprise an AR-LBD unit cell.

An AR-LBD structure includes the secondary or three-dimensional structure of a native AR-LBD, a derivative AR-LBD, or a mutant AR-LBD. Thus, a crystalline form includes native crystals, derivative crystals, and co-crystals. The crystals generally comprise a substantially pure AR-LBD in crystalline form. It is understood that the AR-LBD structures of the invention are not limited to a naturally occurring or native AR-LBD but include polypeptides with substantial sequence identity to an AR-LBD. An AR-LBD structure also includes mutants of a native AR-LBD obtained by replacing at least one amino acid residue in a native AR-LBD with a different amino acid residue, or by adding or deleting amino acid residues within the native polypeptide, and having substantially the same secondary or three-dimensional structure as the native AR-LBD from which the mutant is derived i.e. having a set of atomic structural coordinates that have a root mean square deviation of less than or equal to about 5, 4, 3, 2, or 1.5 Å when superimposed with the atomic structure coordinates of the native AR-LBD from which the mutant is derived when at least 50% to 100% of the atoms of the native AR-LBD are included in the superimposition. It should be noted that the AR-LBD structures contemplated herein need not exhibit AR-LBD activity.

A derivative AR-LBD structure of the invention comprises an AR-LBD structure in association with one or more moieties that are heavy metal atoms. For example, derivative crystals of the invention generally comprise a crystalline AR-LBD in covalent association with one or more heavy metal atoms. The AR-LBD may correspond to a native or mutated AR-LBD. Heavy metal atoms useful for

providing derivative AR-LBD structures include by way of example, and not limitation, gold, mercury, etc.

The invention features an AR-LBD structure in association with one or more moieties that are ligands. The association may be covalent or non-covalent. Crystalline forms of this type are referred to herein as co-crystals. The compound may be any organic molecule, and it may modulate the function of an AR-LBD by for example inhibiting or enhancing its function, or it may be a substrate for the AR-LBD. It is preferred that the geometry of the compound and the interactions formed between the compound and the AR-LBD provide high affinity binding between the two molecules.

The secondary or three-dimensional structures of the particular AR-LBD described herein provide useful models for the secondary or three-dimensional structures of AR-LBD from any species, particularly mammalian, including bovine, ovine, porcine, murine, equine, preferably human, from any source whether natural, synthetic, semi-synthetic, or recombinant.

In a particular embodiment of the invention, a secondary or three-dimensional crystal structure of an AR-LBD that associates with an inhibitor of an AR-LBD is provided comprising at least two or three atomic contacts of atomic interactions in Figure 4, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the inhibitor, and an atomic contact (more preferably, a specific amino acid residue where indicated) on the AR-LBD (i.e. ligand atomic contact). The binding domain may be defined by the ligand atomic contacts of atomic interactions in Figure 4. Preferably, the binding domain is defined by the atoms of the ligand atomic contacts having the structural coordinates for the atoms listed in Table 4.

IDENTIFICATION OF HOMOLOGUES

The knowledge of an AR-LBD structure of the invention enables one skilled in the art to identify homologues of AR-LBD. This is achieved by searches of three-dimensional databases. Since structural folds are conserved to a greater extent than sequence, one may identify homologues with very little sequence identity or similarity. Programs that provide this type of database searching are known in the art and include Dali. The structural coordinates of a protein structure are submitted and the program performs a multiple structural alignment with proteins in the protein data bank. Homologues identified in accordance with the present invention may be used in the methods of the invention described herein.

PROGESTERONE (PR) RECEPTOR

The present invention also provides experimentally isolated crystals for the PR-LBD in complex with the ligand metribolone (R1881). From these experimentally isolated crystals, a three dimensional (3-D) structure for the PR receptor has been produced to medium resolution. The PR-LBD comprises a LBD which is substantially the same as the LBD of the AR-LBD except that the LBD comprises a stronger bending of the helices H10 and H11 and helix H9 has a length which is at least one helical turn shorter than the AR-LBD. The sequence for the wild type PR-LBD site comprises at least SEQ ID No 3 (see Figure 1). The PR-LBD-R1881 crystal complex belongs to the space group $P2_1$ and having the unit dimensions a = 58.40Å, b = 65.0Å, c = 71.18Å and an angle β of 95.7° and with the unit cell dimensions as presented in Table 1.

The present invention also demonstrates the surprising finding that the two independent molecules in the crystal structure of hPR LBD-R1881 exhibit different modes of ligand binding. One orientation pf R1881 in one monomer resembles that of R1881 in the hAR LBD complex while in the second monomer R1881 is orientated similar to progesterone in the hPR LBD-progesterone

complex. Thus it may be possible to design ligands that selectively bind to either one or both of the monomers in the hPR-LBD-ligand complex, thereby dissociating desirable preventative and/or therapeutic effects from undesirable side effects of PR ligands.

A partial homology model of the AR receptor has been created based on the experimentally derived hPR-LBD-progesterone crystal complex. This homology model captures the essential difference in binding between the AR-LBD crystal and AR-LBD model structures. This homology model also highlights the differences with respect to the secondary structure alignment between the model structure of the present invention and that from other published models.

By way of example, the model structure of the present invention differs from other published models [Yong, 1998] with respect to the secondary structure alignment. Yong [1998] based their model on the crystal structure of the RARα LBD [Bourguet, 1995]. The secondary structure assignment by Yong *et al.* as compared to the hAR LBD crystal structure is similar between helices H3 and H10, but the assignment differs most for helices H11, H12 and the additional helix at the C-terminal end.

The ligand binding pocket interactions of the present invention have been determined using the hAR LBD-R1881 crystal structure and the hPR LBD-R1881 complex.

Based on a comparison of the LBP interactions, the differences in ligand binding specificities between the AR and PR can be determined. Using these differences, the ability of a ligand to bind to either or both of the AR and PR may be predicted. Hence, if it is known that one tissue possesses solely one form of an AR and/or PR receptor, then it may be possible to confer a degree of tissue specificity to a ligand by designing a ligand to bind the predominant form of the AR and/or PR present in that tissue.

Thus, the present invention also provides an understanding of the differences between R1881 and progesterone binding to AR and PR receptors and therefore a means to design AR and PR ligands with the desired degree of efficacy.

The present invention also provides a crystal model comprising the hPR-LBD which is built from all or part of the crystal co-ordinate data as shown in Table 5 (see Figure 7).

The present invention also covers these novel aspects and their uses. In this respect, the teachings of the AR-LBD (i.e. hAR-LBD) are equally applicable to the novel aspects of the PR-LBD (i.e. hPR-LBD).

Thus, for example, aspects of the present invention concerning PR-LBD relate to;

A crystal structure comprising a PR-LBD.

A crystal structure for PR-LBD.

A crystal PR-LBD having the structural co-ordinates as set forth in Table 5.

Acrystal structure comprising a PR-LBD-ligand complex.

A crystal structure comprising a PR-LBP.

A model of at least part of an PR-LBD made using or comprising or depicting a crystal structure according to any one of the foregoing aspects of the invention. The crystal structure and the model may be provided in the form of a computer readable medium.

A method of screening for a ligand capable of binding an androgen receptor binding domain, comprising the use of a crystal structure or a model of PR-LBD. For example, the method may comprise the step of contacting the PR-LBD with a test compound, and determining if said test compound binds to said ligand binding domain. The method may be an *in vitro* method and/or an *in silico* method and/or an *in vivo* method.

A ligand identified by a screening method of a foregoing aspect of the invention. Preferably the ligand is capable of modulating the activity of a PR-LBD. As mentioned above, ligands which are capable of modulating the activity of PR-LBDs have considerable therapeutic and prophylactic potential.

The use of a ligand according to the foregoing aspect of the invention, in the manufacture of a medicament to treat and/or prevent a disease in a mammalian patient. There is also provided a pharmaceutical composition comprising such a ligand and a method of treating and/or preventing a disease comprising administering the step of administering such a ligand according or pharmaceutical composition to a mammalian patient.

The crystal structures and models described above also provide information about the secondary and tertiary structure of PR-LBDs. This can be used to gleen structural information about other, previously uncharacterised polypeptides. Thus, according to one aspect of the invention there is provided a method of determining the secondary and/or tertiary structures of polypeptides with unknown (or only partially known) structure comprising the step of using such a crystal or model. The polypeptide under investigation is preferably structurally or functionally related to the progesterone receptor ligand binding domain. For example, the polypeptide may show a degree of homology over some or all parts of the primary amino acid sequence. Alternatively, the polypeptide may

perform an analogous function or be suspected to show a similar binding mechanism to the PR-LBD.

EXAMPLES

The invention will now be further described only by way of example in which reference is made to the following Figures:

Figure 1 which shows a sequence listing for hAR-LBD (SEQ ID No 1) and HPR LBD (SEQ ID No 3) amino acid sequences and a secondary structure for hAR-LBD (SEQ ID No 2). SEQ ID No 1 is presented in the second line of Figure 1. SEQ ID No 3 is presented as the first line in Figure 1. SEQ ID No 2 is presented as the third line in Figure 1.

Figure 2 which shows chemical formulae;

Figure 3 which shows three dimensional structures of hAR LBD and hPR LBD complexed with metribolone (R1881);

Figure 4 which shows a stereo diagrams showing interactions between a bound ligand and protein chain in hAR-LBD and hPR-LBD ligand complexes;

Figure 5 which shows a stereo diagram showing the location of hAR-LBP pathogenic mutations;

Figure 6 which presents Table 4, which has the structural co-ordinates for the hAR-LBD; and

Figure 7 which presents Table 5, which has the structural co-ordinates for the hPR-LBD.

In more detail:

Figure 1 shows a comparison between hAR LBD and hPR LBD amino acid sequences. The numbering scheme of AR is according to [Lubahn, 1988]. The sequence alignment was performed with CLUSTALW [Thompson, 1994]. The residue number applies to the residue directly above or below the last digit. Identical residues are outlined in solid black boxes; gray shading denotes the residues not located in the electron density and thus not included in the model. Selected secondary structure elements are from PROCHECK [Laskowski, 1993] according to Kabsch & Sander [Kabsch, 1983]: E, strand in β-sheet; H, α-helix; Amino acids interacting with bound ligands (R1881 or progesterone) are coloured red (van der Waals cutoff distance 4.0 Å). The mutations presently known for AIS in the hAR LBD are marked below the appropriate position of the respective amino acid in the hAR LBD. Abbreviations: x = prostate cancer, p = PAIS/MAIS, c = CAIS, a = PAIS/MAIS and CAIS, b = PAIS/MAIS and prostate cancer, v = CAIS and prostate cancer, w = PAIS/MAIS and CAIS and prostate cancer.

Figure 2 shows the numbering scheme of R1881 (left) and progesterone (right).

Figure 3 shows the diagrams of the three-dimensional structures of hAR-LBD and hPR-LBD complexed with R1881. (A) MOLSCRIPT/Raster3D [Kraulis, 1991; Merritt, 1994] ribbon diagram of hAR LBD. (B) MOLSCRIPT Stereoview of the C^{α}-trace of the superimposed hAR LBD R1881 (black) and hPR LBD R1881 (red) structures showing the hAR-LBD residue numbering. The (B) view is related to (A) by a clockwise 90° rotation about the vertical axis.

Figure 4 shows the stereo diagrams showing the interactions between the bound ligand and the protein chain in hAR LBD - R1881 (**A**), hPR LBD - R1881 (molecule B) (**B**) and hPR LBD - progesterone (**C**). Residues included are either hydrogen-bonded or have Van der Waals contacts (cutoff distance 4.0 Å) with

any of the ligands. Residues V685, Y763 in hAR LBD and corresponding residues I699, Y777 in hPR LBD are hydrogen-bonded to other residues or water molecules near the ligand binding site and are also included. Bound ligand is coloured black, conserved residues are coloured gray, different residues in hAR LBD and hPR LBD are coloured red. Residue labels with an asterisk (*) denote residues that do not have Van der Waals contacts within the specified cutoff distance with the ligand. Hydrogen bond distances for the hPR LBD - progesterone complex were calculated from the PDB deposited coordinates of molecule A. Figures produced with MOLSCRIPT [Kraulis, 1991].

Figure 5 shows the stereo diagram showing the location of the hAR LBP pathogenic mutations: the coloured spheres are represented at the residue's C^{α} position: mutations observed in prostate cancer (PC) are represented in red, those observed for CAIS are shown in yellow and those observed for PAIS/MAIS are drawn in cyan. Mutation of one residue (Met 749) is implicated in both prostate cancer and CAIS and is represented in orange. Figure produced with MOLSCRIPT [Kraulis, 1991] and Raster3D [Merritt, 1994]. The view is rotated by about 80° clockwise about a vertical axis with respect to the orientation shown in Figure 3A.

Example 1

Plasmid constructs

The cDNAs coding for the human androgen and progesterone receptors were obtained from the groups of A. Cato (Forschungszentrum Karlsruhe, Germany) and P. Chambon (IGBMC, Strasbourg, France) respectively. The ligand binding domains (LBD) of the androgen receptor (amino acid residues (aa) 663 – 919) and the progesterone receptor (aa 678 – 933) were amplified by the PCR technology using appropriate primers and cloned into a pGEX-KG vector [Hakes, 1991]. The resulting fusion proteins consisted of a glutathion-S-transferase,

containing a C-terminal thrombin cleavage site, optimised by a glycine-rich "linker" region followed by the corresponding LBD. The constructs were then transformed into the *E. coli* strain BL21 (DE3).

Protein expression and purification

Fermentation using the corresponding recombinant *E.Coli* strains expressing hAR LBD was carried out in 2XYT medium in the presence of ampicillin (200 ug/ml) supplemented with 10uM R1881. Expression was induced with 30 μM IPTG (isopropyl-β-D-thiogalactoside) and the fermentation (10 L) was continued at 15°C for 14 – 16 hours. Cells were harvested by centrifugation and disrupted twice in a continuous high pressure homogeniser (9000PSI) in a buffer containing 50 mM Tris/HCl, pH 8, 150 mM NaCl, 5 mM EDTA, 10 % Glycerol, 100 uM R1881, 100 uM PMSF and 10 mM DTT. All buffers were purged with nitrogen before adding DTT. The supernatants from ultracentrifugation were loaded onto a glutathione sepharose column, washed with 50 mM Tris_HCl, pH 8, 150 mM NaCl, 5 mM EDTA, 10 % Glycerol, 10 uM R1881, 0.1% n-octyl-β-glucoside and 1 mM DTT and the fusion protein was eluted using the same buffer supplemented with 15 mM reduced glutathione. The eluate was diluted with 100 mM HEPES pH 7.2, 150 mM NaCl, 0.5 mM EDTA, 10% glycerol, 10 uM R1881, 1 mM DTT and 0.1% n-octyl-β-glucoside up to a fused protein concentration of 1 mg/ml. A thrombin cleavage (2 N.I.H. units/mg fusion protein) was performed overnight at 4°C. The protein mixture was further diluted three fold with 10 mM HEPES pH 7.2, 10% glycerol, 10 nM R1881, 10 mM DTT and 0.1% n-octyl-β-glucoside and loaded onto a Fractogel SO_3^- column and eluted with a gradient of 50-500 mM NaCl in a 10 mM HEPES buffer pH 7.2, 10% glycerol supplemented with 10 nM R1881, 10 mM DTT and 0.1% n-octyl-β-glucoside. Approximately 2.4 mg of purified hAR LBD can be recovered from 1L *E.Coli* cell cultures. Protein concentration was determined with Bio-rad Protein Assay. Fermentation and

purification of the hPR LBD was performed identically but a HEPES buffer pH 7.3 was used from the beginning.

Results 1

Protein expression and purification

Glutathion-S-transferase fusion proteins can be expressed to very high levels in the *E. coli* strain BL 21 (DE3) [Hakes, 1991]. We and others have used this system successfully for the production of the ligand binding domains of the human progesterone [Williams, 1998] and androgen receptors. An optimal and stable expression of soluble fusion proteins strongly depends on the presence of ligand in the cells during fermentation (data not shown). During cell disruption, purification and concentration any protein oxidation was avoided. Therefore all buffers were purged carefully with nitrogen and DTT was used as an antioxidant. Fusion proteins were purified by the use of Glutathion sepharose and subsequently cleaved with thrombin. Ligand binding domains were separated from the cleavage products and thrombin by cation exchange chromatography. Concentration was performed with the aid of a nitrogen pressure diafiltration system and the concentrate was immediately used for crystallisation experiments.

Example 2

Crystallisation and data collection

Both proteins were dialysed after purification with buffer containing 50mM HEPES pH 7.2 for hAR LBD, or 10mM HEPES pH 7.2 for hPR LBD, respectively, 10% glycerol, 10mM DTT, 0.1% n-octyl-β-glucoside, 10mM R1881 and 150mM Li_2SO_4 and were concentrated up to 3 mg/ml for the hPR LBD – R1881 and up to 4.4 mg/ml for the hAR LBD – R1881 respectively. Both proteins were crystallised using the vapour diffusion method at 20°C for the hAR

LBD complex and at 4°C for hPR LBD complex respectively. Due to the instability and continuous precipitation of both proteins, crystallisation experiments had to be set up immediately after concentration. For the hAR LBD - R1881 complex, the reservoir solution contained 0.4M $Na_2HPO_4 \cdot 2(H_2O)$, 0.4M K_2HPO_4, 0.1M TRIS-HCl pH 8.5, 0.1M $(NH_4)_2HPO_4$ and 5% PEG200. Drops were composed of equal volumes of protein and reservoir solution and were set up using the sitting drop method. Within two days crystals appeared and grew to typical dimensions of 50x50x80 μm^3 surrounded of precipitate. Crystals were flash frozen using a cryoprotecting solution of 60% PEG 400 in 0.1M TRIS-HCl pH 8.5. Data was collected from one crystal at the ESRF (Grenoble, France) at beamline ID14-EH4 to a resolution of 2.4 Å. For the hPR LBD - R1881 complex, the reservoir solution contained 10% iso-propanol and 100mM sodium citrate in 50mM HEPES pH 7.5. The drops were set up using the hanging drop method and were composed of a 2:1 ratio of protein and reservoir solution. First crystals appeared after five weeks and grew to a size of approximately 160x120x40 μm^3. One crystal was flash frozen using a cryo-protecting solution containing 30% glycerol. Data were collected at beamline BM14 at the ESRF (Grenoble, France) to a resolution of 2.8 Å. Before data collection was complete the crystal decomposed in the X-ray beam.

Both data sets were integrated and reduced using DENZO and SCALEPACK [Otwinowski, 1997]. Statistics of X-ray data collection and processing are summarised in **Table 1**

Table 1. Summary of data collection, processing and scaling

	hAR LBD - R1881	hPR LBD - R1881
Space group	$P2_12_12_1$	$P2_1$
Unit cell	a=54.28 b=66.14 c=71.72 Å	a=58.40 b=65.01 c=71.18 Å β=95.7°
Wavelength (Å)	0.9324	0.9537
Resolution range (Å)	24.4-2.40	12.47-2.80
$N_{observations}$	37,443	67,655
$N_{reflections}$	10,638	8,875
% Completeness *	99.8 (99.9)	67.0 (68.8)
Redundancy	3.5	7.6
R_{merge}*	0.078 (0.351)	0.048 (0.151)
I/σ(I)	12.0	15.2
Estimated $B_{overall}$	49.4	48.2

- Values in parentheses refer to the last resolution shell, 2.46 ≥ d ≥ 2.40 Å for hAR LBD - R1881 complex and 2.87 ≥ d ≥ 2.80 Å for hPR LBD - R1881 complex.

Structure determination

Contrary to the hPR LBD - progesterone complex which crystallises with one homodimer in the monoclinic space group $P2_1$ the hAR LBD crystallises with one monomer in the orthorhombic spacegroup $P2_12_12_1$. Therefore the structure determination for the hAR LBD – R1881 complex was carried out using the molecular replacement method in AMoRe [Navaza, 1994] with the coordinates of only the monomer A of the hPR LBD dimer (PDB entry: 1A28, [Williams, 1998]) without the progesterone ligand. The hPR LBD - R1881 complex crystallises in the same monoclinic space group $P2_1$ and with similar cell constants as the hPR LBD - progesterone complex and thus the whole dimer without the ligand was used as a search model in AMoRe. Clear solutions were obtained for both structures using data between 15.0 and 3.5 Å for the hAR LBD and 12.0 and 3.5 Å for the hPR LBD, respectively.

Refinement of hAR LBD - R1881 complex

The molecular replacement solution obtained was refined using X-PLOR [Brünger, 1992]. In all refinements and map calculations with X-PLOR a bulk solvent correction was used and all low resolution data was included. Prior to the refinement calculations, a random 5% sample of the reflection data was flagged for R-free calculations [Brünger, 1992]. All model interactive visualisation and editing was carried out using TURBO [Roussel, 1990]. Refinement started using data up to 3.5 Å and resolution was gradually extended to 2.4 Å. The model was edited according to the known hAR LBD sequence [Lubahn, 1988] using $2|F_o|-|F_c|$ and $|F_o|-|F_c|$ maps calculated at 3.2 Å resolution and simulated annealed omit maps. The fast wARP [Lamzin, 1997 ; Perrakis, 1997] molecular replacement protocol was also applied after each XPLOR refinement to further improve the $2|F_o|-|F_c|$ electron density map. Prior to its inclusion in the model, the electron density for the R1881 ligand was clearly visible in all maps. A model for the ligand was obtained from the Cambridge Structural Database entry HMESTR [Precigoux, 1981; Allen, 1979]. The XPLOR topology and parameter dictionaries were built using program XPLO2D [Kleywegt, 1995]. In the final refinement at 2.4 Å, 26 water molecules were included in the model, and individual restrained B-factors were refined for all non-hydrogen atoms. The final values of R and R-free were 21.0 % and 29.7 %, respectively. The R-free/R ratio is only slightly smaller than expected [Tickle, 1998] for the number of atoms and reflections used in the refinement. The refinement results and statistics are shown in Table 2.

Table 2. Final refinement statistics for hAR LBD and hPR LBD complexed with R1881

* calculated with SIGMAA [Centre, 1999 ; Read, 1986].

R1881 in complex with	hAR LBD	hPR LBD
Final R-factor (%)	21.0	21.7
Final R-free (%)	29.7	34.3
Number of non-hydrogen protein atoms	2044	4027
non-hydrogen protein atoms missing	22	32
non-hydrogen ligand atoms	21	42
solvent molecules	26	1
Estimated overall r.m.s. coordinate error (Å) *	0.47	0.53
Model r.m.s. deviations from ideality:		
Bond distances (Å) / Bond angles (°)	0.01 / 1.7	0.02 / 4.4
Average B values (Å^2):		
Main-chain / Side-chain	48.3 / 52.1	33.2 / 28.7
Ligand / Solvent	45.2 / 49.2	10.2 / 3.6

Refinement of hPR LBD - R1881 complex

The molecular replacement solution obtained was refined using REFMAC [Murshudov, 1997] using the maximum-likelihood approach. Bulk solvent scaling of Fo and Fc was applied based on Tronrud's solvent correction and all available data with no sigma cut-offs were used. All map calculations were done including calculated F-values for missing reflections. To avoid model bias, calculated maps using only Fo were checked. After the first refinement step the sigmaA-weighted calculated $2|F_o|-|F_c|$ and $|F_o|-|F_c|$ maps were inspected using the program O [Jones, 1991] and electron density of the ligand was clearly observed. The ligand was build up in SYBYL6.5 (Tripos Inc., 1998) and was included in further refinement steps. A dictionary file for distance restraints for the R1881 molecule was prepared using MAKEDICT [Collaborative Computational Project Number 4, 1994]. The model was furthermore refined with alternating cycles of interactive model building and iterative refinement steps. Towards the end of the refinement, only one water molecule in the LBP was added. Although some more possible water sites were located in the electron density we decided not to include

them in the model due to the low resolution and missing data. The final model comprises 4027 protein atoms, 42 ligand atoms and 1 water molecule with final R values of R = 21.7 % and R-free = 34.3 %, respectively. A summary of the refinement and model statistics is included in Table 2.

Results 2

Structure analysis and comparison of the hAR LBD - R1881 and the hPR LBD – R1881 complexes

Both crystal structures were analysed with PROCHECK [Laskowski, 1993] and their stereochemical quality parameters were within their respective confidence intervals. In the Ramachandran φ,ϕ plot for the non-proline and non-glycine residues (not shown) 87.7% for the hAR LBD - R1881 and 85% for the hPR LBD - R1881 structures respectively lie within the most favoured regions. For the hAR LBD - R1881 complex no residue is outside the normally allowed regions whereas in the hPR LBD - R1881 complex two residues are located in disallowed regions (Asn 705 and Ser 793 in molecule A) and three residues (Thr 796 in molecule A, Asn 705 and Ser 793 in molecule B) are located in generously allowed regions. These residues are not involved in ligand binding and are located in loop regions which are most probably not involved in ligand recognition. In the hAR LBD - R1881 structure there is only one close contact (2.6 Å) between Met895 and Ala896 carbonyl oxygens. In the hPR LBD - R1881 structure some close contacts were observed but due to the resolution and completeness of the data this is not surprising. The overall fold of the hAR and hPR LBD - R1881 structures is very similar, and also with that of hPR LBD complexed with progesterone [Williams, 1998]. On the basis of the secondary structure calculated with PROCHECK [Laskowski, 1993] according to Kabsch & Sander [Kabsch, 1983], the hAR LBD - R1881 structure contains 9 α-helices, two 3_{10} helices and four short β-strands associated in two anti-parallel β-sheets. The helices are arranged in the typical 'helical sandwich' pattern as in hPR LBD –

progesterone complex [Williams, 1998] and helices H4, H5 and H10, H11 are contiguous. There are a few minor variations in secondary structure between hAR LBD - R1881 and hPR LBD - progesterone but probably the most interesting is that in hAR LBD - R1881 helix H12 seems to be split into two shorter helical segments, with nine and five residues each respectively. This observation was not seen in the hPR LBD - R1881 structure, although a bending of helix H12 is also seen here. Figure 1 shows a comparison between the amino acid sequences of hAR LBD and hPR LBD. A ribbon diagram of the hAR LBD - R1881 structure is shown in Figure 3 along with a superimposed C^{α}-trace of the hAR LBD - R1881 and hPR LBD - R1881 molecules. The crystal structure coordinates of hAR LBD - R1881 were superimposed with those of hPR LBD - R1881 (molecule B) and hPR LBD - progesterone (molecule A) using LSQKAB [Kabsch, 1976]. For the superposition the main chain atoms except three N-terminal (Cys 669-Pro 671) and one C-terminal (Thr 918) residues were used. The r.m.s. coordinate deviations were 1.16 and 1.22 Å respectively, again an indication of the similarity of the overall fold of these three molecules. In hAR LBD - R1881, Cys 669 and Cys 844 are very close and a disulphide bridge between them was modelled, based on the electron density. However there is no supporting biochemical evidence so far and it should be noted that the temperature factors of both cysteine residues and the adjacent residues are very high. A *cis* peptide bond is found at position Pro 849 in hAR LBD - R1881.

Example 3

Comparative modeling

A model of the hAR LBD was built based on the coordinates of the hPR LBD – progesterone complex (molecule A) [Williams, 1998]. Amino acid substitutions were made based on the sequence alignment in Figure 1 using the Insight 98.0 software (MSI Inc., San Diego, CA USA 1998). Water molecules as observed in the hPR LBD crystal structure (molecule A) were included in the calculations.

Soaking of the initial model and the energy minimisation protocols applied are described in detail elsewhere [Letz, 1999].

Results 3

Comparison of model and crystal hAR LBD structure

The model and the crystal structure of the hAR LBD are very similar with respect to their overall structure, the ligand binding pocket (LBP) and the ligand orientation. The root-mean-square (r.m.s.) deviation between 149 equivalent C^{α} atoms in helices between the model and crystal structure of the hAR LBD is 1.09 Å. It is comparable to the r.m.s. deviation of 0.84 Å and 0.85 Å between the crystal structures of the hAR LBD and the hPR LBD – progesterone complex, on which the model of the hAR LBD was based on and the hAR LBD model and the hPR LBD - progesterone crytsal structure, respectively. The most striking difference between the model and the crystal structure was found in the region of helix H6. In the hAR LBD crystal structure, this region was identified as an α-helix (calculated with the Kabsch & Sander algorithm [Kabsch, 1983] as implemented in Insight98.0 (MSI Inc., San Diego USA, 1998), whereas in the hPR LBD - progesterone complex (molecule A) no α-helix is observed. There is also no α-helix in the hAR LBD model in this area. The ligand orientation in both the hAR LBD - R1881 model and crystal structure is very similar. The same hydrogen bonds are found between the O3 of R1881 and Arg 752 with a distance of 3.0 Å in the crystal and 3.4 Å in the model structure, respectively. In the ligand D-ring, O17 is within hydrogen bond distance to Asn 705 and Thr 877, 3.1 and 3.0 Å in the crystal structure, 2.6 and 3.3 Å in the model structure, respectively.

Discussion

Comparative modelling

The model of the hAR LBD which is based on the hPR LBD - progesterone complex is very similar to the hAR LBD crystal structure with respect to the overall fold and ligand orientation. The most striking differences were a stronger bending of helices H10 and H11 in the model compared to the crystal structure of the hAR LBD. We modelled helix H9 with the same length as in the crystal structure of the hPR LBD - progesterone complex. In the hAR LBD crystal structure it is one helical turn shorter. This region is far away from the LBP and therefore has no influence on the size of the LBP. Our model structure differs from other published models [Yong, 1998] with respect to the secondary structure alignment, as the authors based their model on the crystal structure of the RARα LBD [Bourguet, 1995]. The secondary structure assignment by Yong *et al.* as compared to the hAR LBD crystal structure is similar between helices H3 and H10, the assignment differs most for helices H11, H12 and the additional helix at the C-terminal end.

Ligand binding pocket(LBP) interactions

There are a total of 18 amino acid residues in hAR LBD and hPR LBD that interact with the bound ligand (either R1881 or progesterone). These residues are highlighted in Figure 1 and included in Figure 4. Most of these residues are hydrophobic and interact mainly with the steroid scaffold, while a few are polar and may form hydrogen bonds to the polar atoms in the ligand. The hydrogen-bonding scheme to O3 of R1881 and progesterone is similar but not identical, as shown in Figure 4. In the hAR LBD - R1881 crystal structure, this oxygen atom forms a hydrogen bond to Arg 752 (Arg 766 in hPR LBD), but in contrast with the hPR LBD - progesterone complex the distance of 3.9 Å to Gln 711 (Gln 725 in hPR LBD) does not allow a hydrogen bond. There is a water molecule near O3 that is hydrogen-bonded to three other residues with a nearly triangular geometry (R752 $N^{\eta 1}$, M745 O and Q711 $O^{\varepsilon 1}$ in hAR LBD; R766 $N^{\eta 1}$, M759 O and Q725 $O^{\varepsilon 1}$ in hPR LBD - progesterone). Two of these residues are acceptors, therefore a third acceptor atom (O3 in either progesterone or R1881) in a direction

perpendicular to the plane of the triangle is unlikely, also due to unfavourable geometry. The water molecule hydrogen-bonded to Q711 $N^{\varepsilon 2}$ in hAR LBD (Q725 in hPR LBD) has hydrogen bonds to two other residues (V685 O and F764 O in hAR LBD, I699 O and F777 O in hPR LBD) and in hAR LBD it is hydrogen bonded to a further water molecule, the overall hydrogen bond geometry being nearly tetrahedral. In the hPR LBD – R1881 structure, the ligands in molecules A and B possess slightly different hydrogen bond patterns. In molecule A, O3 of R1881 forms two hydrogen bonds (3.2 Å to Gln 725 $N^{\varepsilon 2}$ and 2.9 Å to Arg 766 $N^{\eta 2}$). One water molecule was located in the F_o-F_c electron density with the same tetrahedral geometry as observed in the hAR LBD - R1881 structure. In molecule B, the ligand is in a slightly different position and the hydrogen bond pattern differs from that observed in molecule A. The O3 of R1881 forms again one hydrogen bond to Arg 766 $N^{\eta 2}$ with a distance of 2.9 Å whereas the distance to Gln725 $N^{\varepsilon 2}$ is now 3.7 Å, outside the acceptable range for a hydrogen bond.

The 17 β hydroxyl group of R1881 forms different hydrogen bonds, when bound to hAR LBD or hPR LBD (Figure 4). In hAR LBD, the 17 β hydroxyl group is hydrogen-bonded to Asn 705 (2.8 Å) and Thr 877 (2.9 Å). The same pattern is observed in molecule B of hPR LBD - R1881 complex where the 17β hydroxyl group of R1881 also forms strong interaction to Asn 719 (2.8 Å), whereas in molecule A the corresponding distance of 3.5 Å is only in the range of a weak interaction. In contrast to the hAR LBD, in both hPR LBD monomers Cys 891 (Thr877 in hAR LBD) shows only a weak interaction with the 17β hydroxyl group of R1881 (3.7 Å in molecule A and of 4.0 Å in molecule B, respectively). However, the relative orientation of the Cys 891 side chain with regard to the hydroxyl group does suggest that this interaction is relevant to the binding of the ligand.

Structural basis for ligand specificity in hAR LBD

The ligand R1881 binds with a relative binding affinity (RBA) of 290 to the wild-type hAR as compared to a value of 180 for DHT and 100 for testosterone, respectively [Teutsch, 1994]. As for the wild-type hPR, the relative binding affinity of R1881 is 190 with respect to progesterone (RBA = 100). Overall, R1881 shows comparable good binding affinities to both receptors, which is also reflected in the orientation of the ligand in the LBPs of the hAR LBD and the hPR LBD (Figure 4). Thr 894 in hPR LBD is replaced by Leu 880 in hAR LBD and the $C^{\delta 2}$ atom of this leucine makes a van der Waals contact (3.9 Å) with the oxygen atom of the 17β hydroxyl group of R1881. This bulkier side chain, along with the substitution of Cys 891 in hPR LBD by Thr 877 in hAR LBD is very likely responsible for the specific recognition of the 17β hydroxyl group of R1881 contrary to the 17β acetyl group of progesterone. Not only there is an extra polar residue (Thr 877 besides Asn 705 which is conserved in AR) which can form an additional hydrogen bond to the 17β hydroxyl oxygen, but the directed decrease in pocket volume caused by the change of Thr894 to Leu880 will very likely inhibit the binding of other bulkier ligands such as progesterone. As previously noted [Williams, 1998] there are no strong hydrogen-bonded interactions between the O20 carbonyl oxygen atom of progesterone and the protein in hPR LBD indicating that the recognition of this group is probably made only through hydrophobic and steric interactions. The hPR LBD can bind R1881 as well as progesterone and, as seen from the above discussion of the hydrogen bonding and van der Waals interaction pattern between protein chain and ligand in the crystal structure, the hPR LBD molecule appears to exhibit two different binding modes for R1881, one resembling that of progesterone (O3 with two hydrogen bonds to the protein chain and the 17β function weakly interacting with the protein chain) and one similar to that of hAR LBD (O3 with only one hydrogen bond to the protein chain and the 17β function also hydrogen bonded to the protein chain). However, these binding modes do not seem to imply significant changes in ligand position and orientation within the LBP.

Mutations

We analysed whether the mutated amino acid residues are predominantly found in the interior of the protein or at the surface. Comparison of the solvent accessibility of these residues revealed that a nearly even distribution is found between buried, medium or fully accessible residues. Table 3 lists all those mutations in or near the AR ligand binding pocket (LBP) which are known to be involved in AIS and prostate cancer (PC), their location with respect to secondary structural elements as well as the potential effect of the mutations.

Table 3: hAR LBD mutations observed in prostate cancer, CAIS and PAIS/MAIS. For convenience, the equivalent positions of the amino acid residues (aar) in the hPR LBD are given. Bold numbers indicate available mutant data in the PR. All mutations are taken from the androgen receptor gene mutations data base (Gottlieb et al. 1998 and references therein)

	Mutation in AR	aar in PR	Location in LBD	Vicinity of ligand	Comment
prostate cancer	Leu701-His	715	H3	D	His: too close contacts to Phe876, hydrophobic environment for His: Met780, Phe876; Leu880
	Met749-Ile	763	H5	A	Ile either too close to Arg752 or Phe764
	Thr877-Ala	**891**	H11	D	No H-bond partner for ligand 17 β OH
	Thr877-Ser	**891**	H11	D	2 energetically favourable conformations for Ser similar to the O^{γ} or C^{γ} position of Thr
	Leu880-Gln	**894**	H11	D	Hydrophobic environment for Gln: Leu 701, Met 780, Phe 876
	Phe891-Leu	**905**	Loop H11/H12	D	Leu side chain too close to Leu881 in the 2 most often observed side chain conformations for Leu
CAIS	Asn705-Ser	**719**	H3	D	Ser: too small for H-bond partner to ligand 17 β OH
	Leu707-Arg	721	H3	A	Arg: too elongated for this area
	Met749-Val	**763**	H5	A	Val: branched aar, C^{γ} too close to ligand
PAIS/MAIS	Gly708-Ala	**722**	H3	C	No hindrance for Ala
	Gly708-Val	**722**	H3	C	Val: too close to Trp 741, Met 895, ligand
	Met742-Val	756	H5	B/C	Val fits into LBP but environment is less tightly packed, the LBP is enlarged
	Met742-Ile	756	H5	B/C	Ile fits into LBP but environment is less tightly packed, LBP is enlarged
	Met745-Thr	759	H5	A	Val too close to ligand
	Val746-Met	760	H5	B	Met too close to Met 741, Leu 873, ligand
	Arg752-Gln	**766**	H5	A	Gln too small for H-bond partner to ligand O3
	Phe764- Ser	778	S1	A	Ser: no stacking with A-Ring of ligand possible
	Met787-Val	801	H7	B	No hindrance for Val, but fewer contacts to Val 746, Leu 873 and ligand

Mutations are reported for 12 of the 18 residues considered to interact with the ligand R1881 within 4.0 Å as discussed above, as well as two additional residues within 5.0 Å of the ligand (G708 and V746 in hAR LBD, G722 and Val760 in hPR LBD). In some cases the same amino acid can be mutated into different residues, e.g. T877A and T877S. For most of these mutations, a structural effect can be associated with the substitution. For example, when Met 749 in hAR LBD is substituted by the branched amino acid valine, the C^{γ} side chain atoms would become too close to the ligand. The location of these mutations in the three-dimensional structure of hAR LBD - R1881 is shown in Figure 5, and it can be seen that the mutations involved in the prostate cancer (PC) cluster mainly near the R1881 17β hydroxyl group while those involved in AIS are arranged mainly around the other parts of the ligand. One notable exception is Met 749 which has mutations implicated in both PC and CAIS and is located in the vicinity of R1881 O3, opposite from the other PC-implicated mutations.

Mutations in the LBP observed in the prostate cancer cell line LNCaP

The prostate tumor cell line LNCaP contains an AR receptor showing a significant increased binding affinity for gestagenic and estrogenic steroids but shows identical R1881 binding (Veldscholte *et al.* 1990). A single point mutation (T877A) is associated with this abnormal behaviour. With an alanine at this position an important hydrogen bond partner for the 17β hydroxyl group in R1881, testosterone or dihydrotestosterone (DHT) would be missing, but the other hydrogen bond partner, Asn 705, involved in ligand binding could still orient the ligand in the LBP. Mutagenesis experiments of hPR emphasised the critical role of this asparagine residue in ligand interaction (Letz *et al.* 1999). In the crystal structure of the hPR LBD – progesterone complex, Cys 891 is found at the position of Thr 877, but no hydrogen bond of the 17β acetyl group of progesterone was observed although Cys 891 is relatively close (4.3 Å in molecule A, 4.4 Å in molecule B) to O20 of progesterone. However, bacterial extracts of a mutated hPR LBD (C891S or C891V) showed a large decrease in

relative binding affinity for progesterone and the purified mutated hPR LBD was completely inactive in binding assays [Letz, 1999].

Mutations in the LBP observed in CAIS

The three mutations in the hAR LBP described for CAIS are substitutions that considerably change the size of the respective amino acid side chains, N705S [Bellis, 1992; Pinsky, 1992], L707R [Lumbroso, 1996] and M749V [Bellis, 1992; Jakubicza, 1992]. This change in size alters the LBP such that the local structure and interactions to the ligand are disturbed.

In the AR LBD and PR LBD crystal structures, Asn 705 or Asn 719 respectively is one of the hydrogen bond partners to the ligand R1881, but not to progesterone. If this residue is substituted to Val in hPR LBD, only a moderate effect was observed on the binding activity of progesterone, considering the K_D and half-life values [Letz, 1999]. In the crystal structure of the hPR LBD - progesterone complex, Asn 719 is involved in the stabilisation of the loop between H11 and H12, via hydrogen bond between Asn 719 $N^{\delta 2}$ and Glu 904 O. In the hAR LBD, an identical stabilisation is found, by means of a hydrogen bond between Asn 705 $N^{\delta 2}$ and Asp 890 O. A N705S mutation, observed in a patient suffering from CAIS would have a two-fold effect, destablilization of the structure and loss of a hydrogen bond partner for the ligand.

In the described hAR mutant L707R, the structure integrity disturbance is also reflected in the binding constants. Considering a van der Waals cutoff distance of 4.0 Å, the side chain of Leu 707 makes close contacts with the A-ring of R1881 as well as five residues in the protein chain: V685, A687, Q711, F764 and L768. The first two residues are located in a loop region between H2 and H3, the third is located within H3 and is involved in the hydrogen bonding pattern of a water molecule near the O3 atom of R1881, and the final two belong to each of the two strands S1 and S2 of the first short β-sheet. Clearly, such a variation in the size of

the side-chain would have a large impact, not only in the LBP but in disrupting the overall protein fold itself. The mutated receptor shows undetectable binding affinity to the ligand R1881 as obtained by Scatchard plot analysis and no transcriptional activity is found [Lumbroso, 1996].

Mutations in the LBP observed with PAIS/MAIS

Seven described mutations in the hAR LBP are associated with PAIS/ MAIS, and multiple substitutions were observed for amino acids at position 708 [Albers, 1997] and 742 [Bevan, 1996]. In the hAR LBD crystal structure, a substitution of Gly 708 to alanine should be tolerated whereas a valine at this position would interfere with ligand binding. The closest distance of the C atom of an alanine residue to the ligand would be 3.0 Å, however, the Cg atoms of a valine would be too close to the ligand atoms (1.5 Å). The substitution of the equivalent Gly 722 in the hPR receptor to serine does not influence the binding of agonists, but rather that of the antagonist RU486 [Benhamou, 1992].

In all steroid receptors, the steroid is stabilised by a hydrogen bond between the A-ring of the ligand and an arginine (Arg 752 in hAR). A smaller amino acid residue at this position (mutation to glutamine in hAR) should have a dramatic impact on ligand binding as the stabilisation of the A-ring would be severely hampered due to the lack of a electrostatic interaction (Cabral *et al.* 1998, Komori, 1998). A similar effect has been reported for the hPR receptor where a mutation (R766H) resulted in a low or even non-detectable binding affinity. The side-chain of histidine is too small to serve as a hydrogen bond partner to the O3 atom in progesterone [Letz, 1999].

In the hAR mutation F764S, R1881 shows a similar binding affinity as the wild type receptor, but a rapid ligand dissociation is observed [Marcelli, 1994]. In the crystal structure, Phe 764 is involved in the stabilisation of the A-ring position. A

smaller amino acid like serine would allow binding of the ligand, but very likely not contribute to the tight binding of R1881.

Mutations M742V or M742I both dramatically reduce the binding affinity of R1881 [Bevan, 1996]. Although Ile and Val fit into the LBP, the changed environment is less tightly packed and the LBP is enlarged, thus affecting the binding of the ligand.

However, not all mutations can be related to a disturbance of the structure. In case of the M787V mutation in the hAR LBD, it was found by Scatchard analysis that R1881 and DHT binding was undetectable or strongly reduced [Nakao, 1992]. The lack of androgen binding was thought to be the cause for AIS. In the crystal structure, a methionine to valine substitution could be tolerated. The lack of binding affinity found for R1881 may account for a destabilisation in the LBP as the Met 787 side chain is in van der Waals contact with other amino acids like Val 760 and Leu 887 as well as ligand atoms.

Example 4

Modified method for isolating hPR-LBD

Purification of hPR LBD with R1881:

The pGEX-KG-hPR LBD construct rather than the pGEX-KG-hAR LBD construct was used for fermentation. As a result, compared to "normal" hPR LBD purification, there were a few differences at the beginning of the purification procedure. These differences were related to the size of the construct and to different pH values, salt and additive concentrations:

Construct	"normal" hPR LBD purification: pGEX-2T-hPR LBD construct (Gly-hPR LBD 677-933), this time: pGEX-KG-hPR LBD: (GSPGISGGGGGI-hPR LBD 678-933) (N-terminal end extended by 10 residues).
pH	Reduction from pH 8.0 to pH 7.3 (instead of pH 7.5)
NaCl	Increase from 200 to 300 mM
EDTA	Increase from 0.5 to 5 mM
DTT	Increase from 5 to 10 mM
R1881	100 µM on lysis and binding to glutathione sepharose column
Urea	Reduction from 2 M to 0 M (purification without urea!)

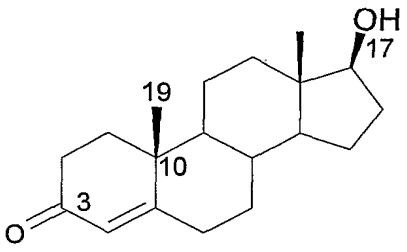
Results 4

Purification was successful and the protein was concentrated to 3 mg/ml (total protein 1.0 mg after SDS PAGE

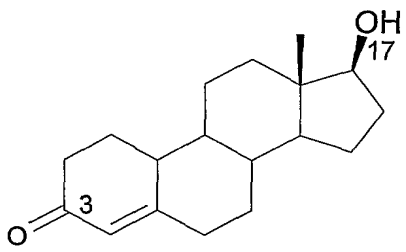
Example 5

HAR-LBD-Ligand complexes

Energy minimisation calculations were performed with the ligands R1881, testosterone and 19Nor-testosterone. In a first step the protocols used in the calculations were optimized such that the energy minimisation calculation of the hAR LBD – R1881 complex reproduced the interactions between the protein and the ligand as observed in the crystal structure of the same complex especially the hydrogen bond partners of the O3 and O17 atoms of the ligand with the protein, i.e. Arg752, Gln711 and Asn705. Then the same protocols were used for the calculations of the hAR LBD – testosterone and the hAR LBD-19Nor-testosterone complexes.



testosterone



19Nor-testosterone

Results 5

The results of the energy minimisation calculations confirm the hydrogen bond interactions at atom O3 of both testosterone and 19Nor-testosterone as observed in the crystal structure between R1881 and the hAR LBD (with Arg752 and Gln711). However, the interaction partners of the O17 atom at the D-ring are different due to the methyl substituent attached to position 10 of the steroid skeleton (position 19).

In case of the ligand 19Nor-testosterone, the O17 atom interacts with the side chain of Asn705. The calculations of the hAR LBD in complex with the ligand testosterone showed a shift in the orientation of the ligand in the ligand binding pocket (LBP) most likely due to the presence of the methyl group attached to position 10 of the steroid scaffold. Here, an interaction of the O17 atom with the side chain of Thr877 is observed in the calculations. The methyl group at that position in the ligand would be too close to amino acid residues Trp741 and Met745. In order to accommodate this ligand in the LBP, the ligand is shifted as well as the side chains of the amino acid residues Trp741 and Met745.

The amino acid residues of the hAR LBD within a radius of 4 Å around the respective ligands are the same for R1881 and 19Nor-testosterone. Due to the slight shift of testosterone of about 1.5 Å in the D-ring area, amino acid residues Trp741 and Ile899 are now farer away from testosterone.

SUMMARY

A crystal comprising an androgen receptor ligand binding domain (AR-LBD) is provided. The crystal structures of the human Androgen Receptor (hAR) in comparison with the human Progesterone Receptor (hPR) Ligand Binding Domains (LBDs) in complex with the same ligand metribolone (R1881) is also provided. The three-dimensional structures of the hAR LBD as well as the hPR LBD show the typical nuclear receptor fold. The change of two residues in the ligand binding pocket (LBP) between hPR and hAR was identified as the most likely source for the specificity of the R1881 ligand binding to hAR LBD. The AR-LBD amino acid residues are Leu 880 and Thr 877. The corresponding PR amino acid residues Thr894 and Cys891. In addition, there are three other amino acid changes which maybe involved in binding of ligands other than R1881. The AR amino acid residues are Gln 783, Met 749 and Phe 876. The PR amino acid residues are Leu 797, Leu 763 and Tyr 890. The structural implications of the 14 known mutations in the LBP of the hAR LBD associated with either prostate cancer or the partial or complete androgen receptor insensitivity syndrome were analysed. The effects of most of these mutants could be explained on the basis of the crystal structure.

In one aspect, the present invention provides a method of identifying a compound that modulates (ie increases or decreases) AR activity, comprising: modeling test compounds that fit spatially into an AR LBD of interest using a model of the AR-LBD or portion thereof, screening the test compounds in an assay, for eg, a biological assay, characterised by binding of a test compound to the LBD and identifying a test compound that modulates AR activity wherein the structural model comprises structural co-ordinates of the LBD amino acid residues: L701; L704; N705; L707; Q711; M742; L744; M745; M749; R752; F764; Q783; M787; F876; T877; L880; F891; M895 or a homologue thereof.

In another aspect, the present invention relates to a computer readable medium having stored thereon a model of a crystal comprising an LBD structure of the AR-LBD.

In a further aspect, the present invention relates to a computer readable medium having stored thereon a model of a crystal comprising an AR-LBD wherein said model is built from all or part of the X-ray diffraction data shown in Table 1 and/or Table 2.

In an even further aspect, there is provided the use of the structural co-ordinates provided in Table 4 for the identification of a ligand or for building a crystal structure for an AR-LBD.

In another aspect, the present invention relates to a computer controlled method for designing a ligand capable of binding to the AR receptor comprising:

(i) providing a model of the crystal structure of the AR-LBD;

(ii) analysing said model to design a ligand which binds to the LBD; and

(iii) determining the effect of said ligand on said AR-LBD.

In a further aspect, there is provided a machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three dimensional representation of a crystal or a homologue of said crystal.

The present invention also provides a computer comprising such a storage medium.

The present invention also provides the use of such a computer in an industrial context, such as identifying putative ligands.

In another aspect, there is provided a method for homology modelling a crystal comprising an AR-LBD or a homologue thereof comprising:

(i) aligning the sequence of the AR-LBD (SEQ ID No 1 or SEQ ID No 2) or an AR-LBD homologue with the AR-LBD sequence and incorporating this sequence into the AR-LBD model;

(ii) subjecting a preliminary AR-LBD model to energy minimisation resulting in an energy minimised model;

(iii) remodeling the regions of said energy minimised model where stereochemistry restraints are violated; and

(iv) obtaining a final homology model.

Various modifications and variations of the described methods and system of the invention will be apparent to those skilled in the art without departing from the scope and spirit of the invention. Although the invention has been described in connection with specific preferred embodiments, it should be understood that the invention as claimed should not be unduly limited to such specific embodiments. Indeed, various modifications of the described modes for carrying out the invention which are obvious to those skilled in chemistry or biology or related fields are intended to be covered by the present invention. All publications mentioned in the above specification are herein incorporated by reference.

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CLAIMS

1. A crystal comprising an androgen receptor ligand binding domain (AR-LBD).

2. A crystal comprising a ligand binding domain (LBD) wherein the LBD is arranged in an α-helical sandwich comprising preferably the α-helices: H1, H3, H4, H5, H6, H7, H8, H9, H10, H11 and H12; preferably two 3_{10} helices; and preferably four short β strands (S1, S2, S3 and S4) associated in two anti-parallel β-sheets;

wherein the helices H4, H5, H10 and H11 are preferably contiguous helices; and

wherein

either helix H6 is preferably an α-helix and/or

helix H12 comprises preferably two helical segments of preferably 9 amino acid residues and preferably 5 amino acid residues.

3. A crystal according to claim 2 wherein the LBD is an AR-LBD.

4. A crystal according to any one of claims 1-3 wherein the LBD is a human AR-LBD.

5. A crystal according to any one of claims 1-4 wherein the LBD comprises the sequence presented as SEQ ID No 1 or a homologue or a mutant thereof.

6. A crystal according to any one of the preceding claims wherein the LBD comprises the secondary structure presented as SEQ ID No 2 or a homologue thereof.

7. A crystal comprising a ligand binding pocket (LBP); wherein the LBP is defined by the following amino acid residue structural co-ordinates: L701; L704; N705; L707; Q711; M742; L744; M745; M749; R752; F764; Q783; M787; F876; T877; L880; F891; M895; or a homologue thereof.

8. A crystal comprising an LBP wherein the LBP is defined by a mutation or substitution or derivatisation in or of any one or more of the structural co-ordinates of the LBD amino acid residues as defined in claim 7.

9. A crystal according to claim 8 wherein the mutation is selected from the group consisting of any one or more of: L701H; M749I; T877A; T877S; L880Q; F891L;N705S; L707R; M749V; G708A; G708V; M742V; M742I; M745T; V746M; R752Q; F764S; M787V; or a homologue thereof.

10. A crystal according to any one of the preceding claims wherein the crystal belongs to the space group $P2_1$, 2_1, 2_1, and having the unit dimensions a = 58.28Å, b = 66.14Å, c = 71.72Å.

11. A crystal according to any one of the preceding claims wherein the crystal further comprises a ligand bound to the LBD or a portion thereof.

12. A crystal according to claim 11 wherein the ligand is metribolone (R1881) or a mimetic thereof.

13. A method of screening for a ligand capable of binding to a LBD wherein the method comprises the use of a crystal according to any one of claims 1-12.

14. A method for screening for a ligand capable of binding to a LBD wherein the LBD is defined in claim 2 and/or claim 3 and/or claim 4 and/or claim 7 and/or

claim 8; the method comprising contacting the LBP with a test compound, and determining if said test compound binds to said LBP.

15. A method according to claim 14 wherein the method is to screen for a ligand useful in the prevention and/or treatment of an androgen related disorder wherein the androgen related disorder is selected from the group consisting of androgen insensitivity syndrome (AIS), partial androgen insensitivity syndrome (PAIS), mild androgen insensitivity syndrome (MAIS), complete androgen insensitivity syndrome (CAIS) and prostrate cancer (PC).

16. A process comprising the steps of:

(a) performing the method according to claim 13 or claim 14 or claim 15;

(b) identifying one or more ligands capable of binding to a LBD; and

(c) preparing a quantity of those one or more ligands.

17. A process comprising the steps of:

a) performing the method according to claim 13 or claim 14 or claim 15;

(b) identifying one or more ligands capable of binding to a LBD; and

(c) preparing a pharmaceutical composition comprising those one or more identified ligands.

18. A process comprising the steps of:

(a) performing the method according to claim 13 or claim 14 or claim 15;

(b) identifying one or more ligands capable of binding to a LBD; and

(c) modifying those one or more identified ligands capable of binding to a LBD; and

(d) performing said method according to claim 13 or claim 14 or claim 15; and

(d) optionally preparing a pharmaceutical composition comprising those one or more modified ligands.

19. A ligand identified by the method of claim 13 or claim 14 or claim 15 wherein the ligand is a LBD binding compound.

20. A ligand according to claim 19 wherein the ligand is capable of interacting with a LBD region located in helices H4 and H5 of the LBD.

21. A ligand according to claim 19 wherein the ligand is capable of interacting with one or more of: Asn 705, Met 749, Gln 783, Phe 876, Thr 877, Leu 880 of an AR-LBD.

22. A ligand according to claim 21 wherein the ligand is capable of interacting with one or more of: Met 749, Gln 783, Phe 876, Thr 877, Leu 880 of an AR-LBD.

23. A ligand according to claim 21 or claim 22 wherein the ligand is capable of interacting with one or more of: Thr 877, Leu 880 of an AR-LBD.

24. A ligand according to claim 19 wherein the ligand is capable of interacting with Asn 705.

25. A ligand according to claim 19 wherein the ligand is capable of fitting spatially into a LBP wherein the LBP is defined by the structural co-ordinates of the mutated amino acid residues L701H; M749I; T877A; T877S; L880Q; F891L;N705S; L707R; M749V; G708A; G708V; M742V; M742I; M745T; V746M; R752Q; F764S; M787V, or a homologue thereof.

26. A pharmaceutical composition comprising a ligand according to any one of claims 21-25 and a pharmaceutically acceptable carrier, diluent, excipient or adjuvant or any combination thereof.

27. A method of preventing and/or treating an androgen related disorder comprising administering an ligand according to any one of claims 21-25 and or a pharmaceutical according to claim 26 wherein said agent or said pharmaceutical is capable of modulating an AR-LBD to cause a beneficial preventative and/or therapeutic effect.

28. A method according to claim 27 wherein the androgen related disorder is that defined in claim 15.

29. Use of a ligand according to any one of claims 21-25 in the preparation of a pharmaceutical composition for the treatment of an androgen related disorder.

30. Use of a crystal comprising an AR-LBD in the preparation of a medicament to prevent and/or treat androgen related disorders.

31. Use according to claim 30 wherein the AR-LBD is used to screen for ligands that can modulate the activity of the AR-LBD.

32. An AR-LBD agonist, wherein the AR-LBD is that defined in any one of claim 1 and/or claim 3 and/or claim 4.

33. An AR-LBD antagonist wherein the AR-LBD is that defined in any one of claim 1 and/or claim 3 and/or claim 4.

34. A crystal comprising an androgen receptor ligand binding pocket (AR-LBP).

35. An AR-LBD in a crystal form.

36. A method for predicting, simulating or modelling the molecular characteristics and/or molecular interactions of a ligand binding domain (LBD) comprising the use of a computer model, said computer model comprising, using, or depicting the structural coordinates of a ligand binding domain as provided in Table 4 or Table 5 to provide an image of said binding ligand domain and to optionally display said image.

37. A method according to claim 36 wherein said method further comprises the use of a computer model comprising, using, or depicting the structural coordinates of a ligand to provide an image of said ligand and to optionally display said image.

38. A method according to claim 37 wherein said method further comprises providing an image of said ligand in association with said LBD and optionally displaying said image.

39. A method according to claim 38 wherein said ligand is manufactured and optionally formulated as a pharmaceutical composition.

40. A crystal substantially as described herein and with reference to the accompanying Figures.

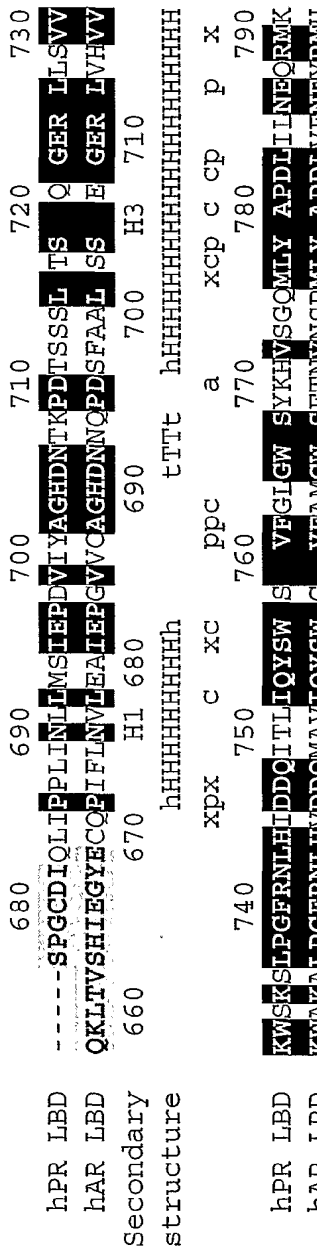


FIG. 1

Mutations presently known for AIS in the hAR LBD are marked below the appropriate position of the respective amino acid in the hAR LBD. Abbreviations: x=prostate cancer, p=PAIS/MAIS, c=CAIS, a=PAIS/MAIS and CAIS, b=PAIS/MAIS and prostate cancer, v=CAIS and prostate cancer, w=PAIS/MAIS and CAIS and prostate cancer

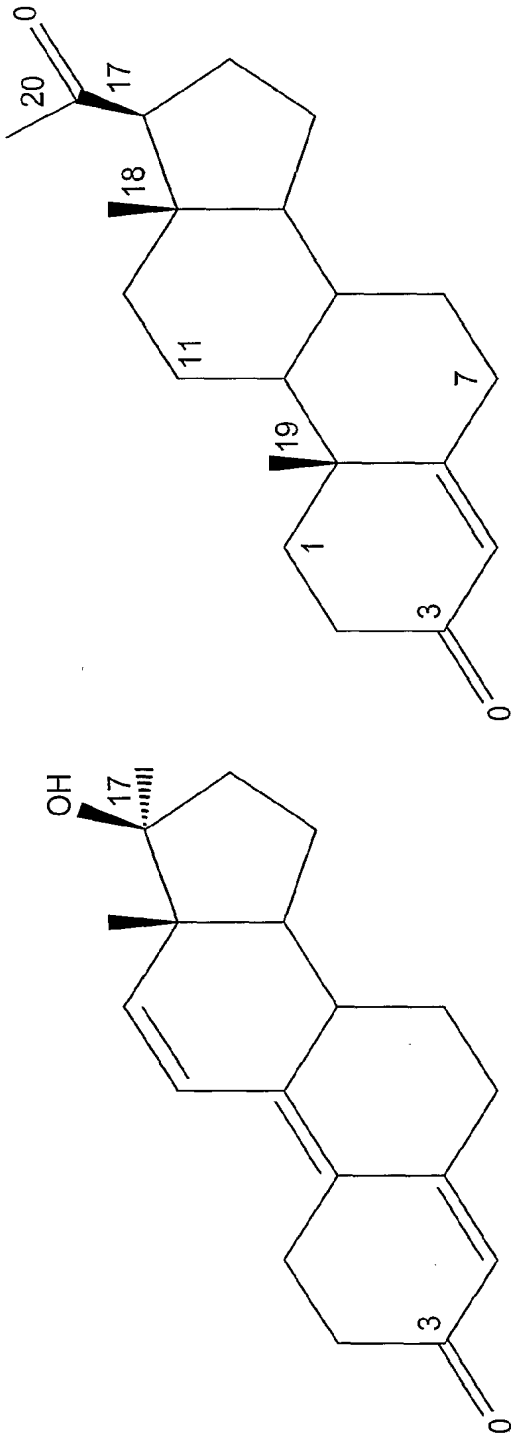


FIG. 2

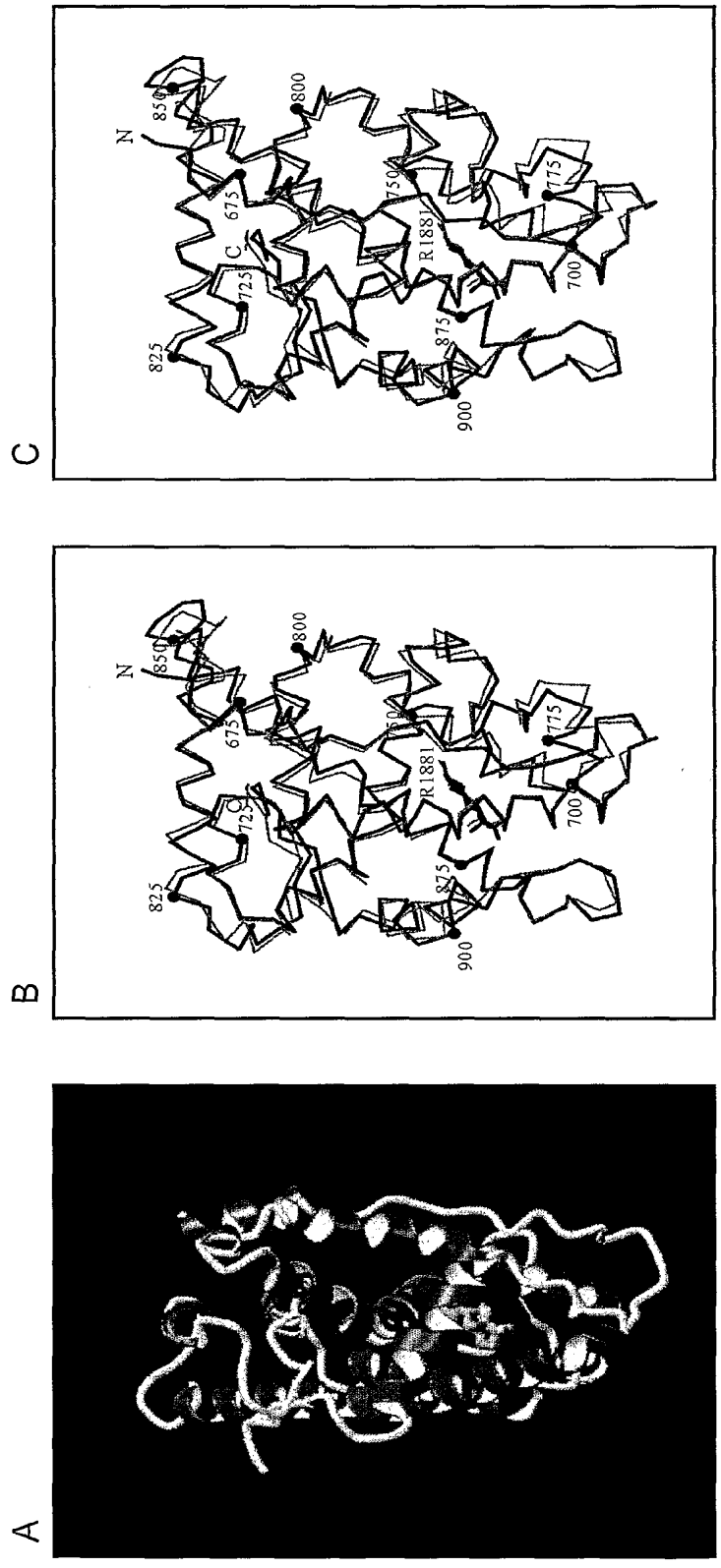
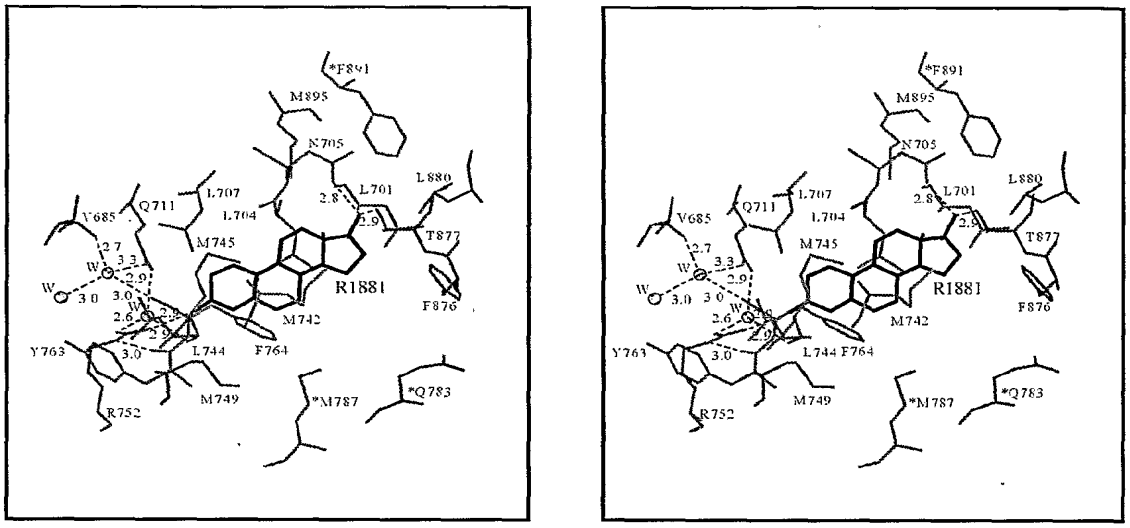
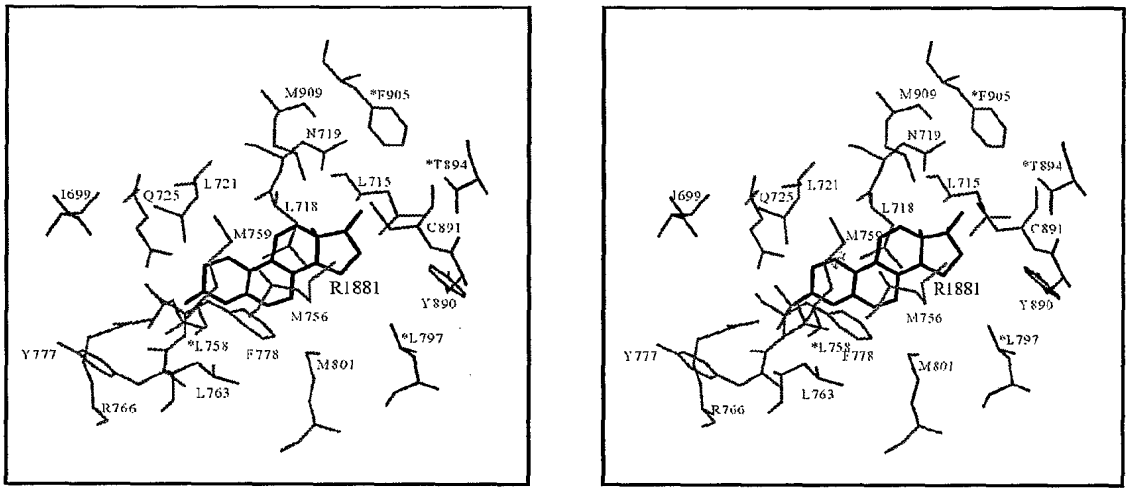

C
N
850
800
675
750
775
C
R1881
725
700
825
875
900
B
N
850
800
675
775
R1881
725
700
825
875
900
A

FIG. 3

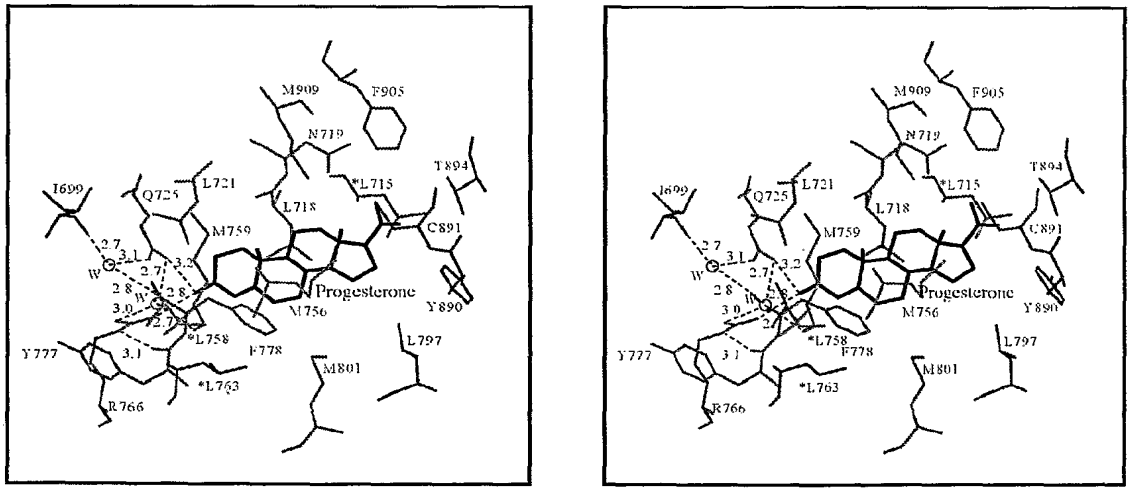
A


*F891
M895
N705
L880
L701
Q711
L707
L704
V685
M745
T877
R1881
F876
M742
Y763
L744
F764
M749
R752
*M787
*Q783

B


M909
*F905
N719
*T894
I699
Q725
L721
L715
L718
M759
C891
R1881
Y890
M756
*L758
F778
*L797
Y777
M801
L763
R766

C


M909
F905
N719
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L721
*L715
L718
M759
C891
Progesterone
Y890
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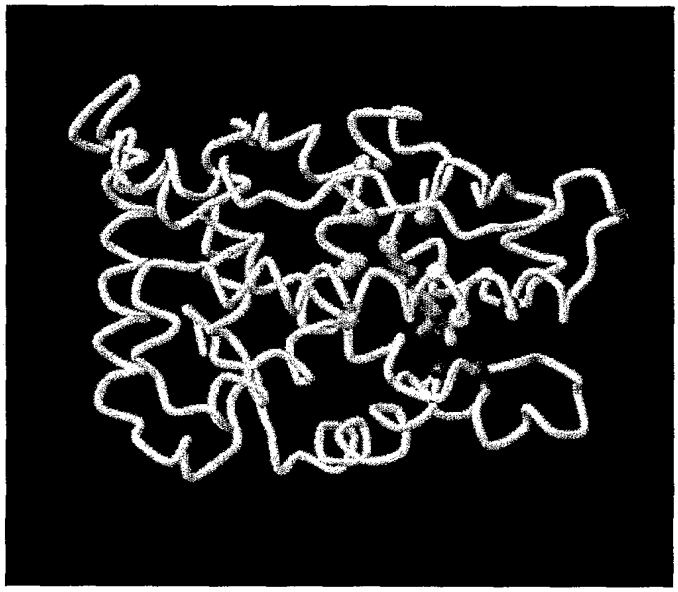
F778
L797
Y777
M801
*L763
R766

FIG. 4



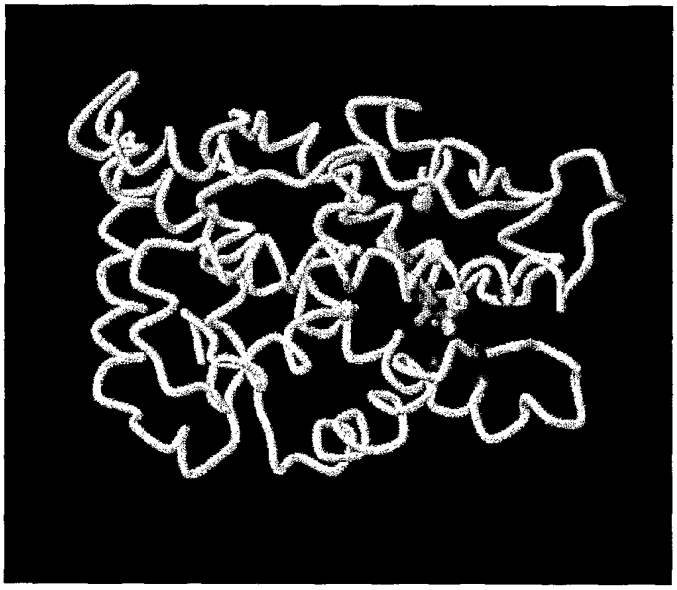


FIG. 5

FIG. 6 (TABLE 4)

coordinates of hAR LBD in complex with the ligand R1881

ATOM	1	C	CYS	669	21.892	8.793	22.633	1.00 86.11	C
ATOM	2	O	CYS	669	22.074	8.565	21.427	1.00 77.81	O
ATOM	3	CB	CYS	669	24.276	9.675	22.802	1.00 88.59	C
ATOM	4	SG	CYS	669	24.838	11.217	21.992	1.00 94.18	S
ATOM	7	N	CYS	669	22.921	9.448	24.884	1.00 77.12	N
ATOM	9	CA	CYS	669	22.859	9.723	23.414	1.00 86.87	C
ATOM	10	N	GLN	670	20.835	8.318	23.308	1.00 87.01	N
ATOM	12	CA	GLN	670	19.841	7.405	22.705	1.00 89.27	C
ATOM	13	CB	GLN	670	19.222	6.498	23.792	1.00 93.96	C
ATOM	14	CG	GLN	670	18.335	5.330	23.282	1.00 90.90	C
ATOM	15	CD	GLN	670	18.946	3.972	23.548	1.00 89.73	C
ATOM	16	OE1	GLN	670	19.840	3.532	22.833	1.00 86.20	O
ATOM	17	NE2	GLN	670	18.456	3.297	24.575	1.00 91.02	N
ATOM	20	C	GLN	670	18.731	8.155	21.935	1.00 86.82	C
ATOM	21	O	GLN	670	18.184	9.157	22.427	1.00 85.28	O
ATOM	22	N	PRO	671	18.312	7.612	20.764	1.00 82.62	N
ATOM	23	CD	PRO	671	18.835	6.381	20.127	1.00 80.30	C
ATOM	24	CA	PRO	671	17.273	8.224	19.921	1.00 76.72	C
ATOM	25	CB	PRO	671	17.414	7.449	18.599	1.00 73.17	C
ATOM	26	CG	PRO	671	17.777	6.058	19.076	1.00 75.93	C
ATOM	27	C	PRO	671	15.795	8.270	20.367	1.00 71.10	C
ATOM	28	O	PRO	671	14.933	8.452	19.508	1.00 75.36	O
ATOM	29	N	ILE	672	15.473	8.187	21.661	1.00 59.44	N
ATOM	31	CA	ILE	672	14.045	8.210	22.043	1.00 57.16	C
ATOM	32	CB	ILE	672	13.792	7.852	23.525	1.00 54.74	C
ATOM	33	CG2	ILE	672	14.835	8.496	24.426	1.00 64.17	C
ATOM	34	CG1	ILE	672	12.353	8.234	23.892	1.00 47.09	C
ATOM	35	CD1	ILE	672	11.963	7.922	25.277	1.00 56.37	C
ATOM	36	C	ILE	672	13.232	9.465	21.682	1.00 59.85	C
ATOM	37	O	ILE	672	12.069	9.358	21.234	1.00 54.31	O
ATOM	38	N	PHE	673	13.834	10.642	21.885	1.00 61.01	N
ATOM	40	CA	PHE	673	13.167	11.909	21.583	1.00 53.54	C
ATOM	41	CB	PHE	673	13.980	13.095	22.129	1.00 55.20	C
ATOM	42	CG	PHE	673	13.247	14.403	22.055	1.00 54.87	C
ATOM	43	CD1	PHE	673	12.248	14.703	22.976	1.00 54.05	C
ATOM	44	CD2	PHE	673	13.491	15.292	21.017	1.00 47.32	C
ATOM	45	CE1	PHE	673	11.500	15.858	22.860	1.00 53.41	C
ATOM	46	CE2	PHE	673	12.749	16.448	20.897	1.00 49.17	C
ATOM	47	CZ	PHE	673	11.749	16.730	21.816	1.00 53.29	C
ATOM	48	C	PHE	673	12.960	12.039	20.068	1.00 44.47	C
ATOM	49	O	PHE	673	11.858	12.376	19.585	1.00 38.12	O
ATOM	50	N	LEU	674	14.023	11.743	19.327	1.00 36.26	N
ATOM	52	CA	LEU	674	13.976	11.789	17.882	1.00 38.85	C
ATOM	53	CB	LEU	674	15.358	11.487	17.303	1.00 45.56	C
ATOM	54	CG	LEU	674	16.279	12.708	17.252	1.00 49.73	C
ATOM	55	CD1	LEU	674	17.687	12.339	16.760	1.00 48.00	C
ATOM	56	CD2	LEU	674	15.638	13.737	16.318	1.00 42.53	C
ATOM	57	C	LEU	674	12.919	10.866	17.273	1.00 38.35	C
ATOM	58	O	LEU	674	12.254	11.238	16.300	1.00 39.82	O
ATOM	59	N	ASN	675	12.731	9.686	17.871	1.00 40.82	N
ATOM	61	CA	ASN	675	11.744	8.705	17.370	1.00 41.39	C
ATOM	62	CB	ASN	675	11.734	7.434	18.209	1.00 51.05	C
ATOM	63	CG	ASN	675	13.008	6.648	18.091	1.00 55.02	C

ATOM	64	OD1	ASN	675	13.672	6.651	17.045	1.00	54.01	O
ATOM	65	ND2	ASN	675	13.370	5.971	19.166	1.00	60.08	N
ATOM	68	C	ASN	675	10.374	9.297	17.456	1.00	39.61	C
ATOM	69	O	ASN	675	9.527	9.092	16.568	1.00	33.60	O
ATOM	70	N	VAL	676	10.159	10.022	18.551	1.00	37.88	N
ATOM	72	CA	VAL	676	8.894	10.687	18.781	1.00	36.37	C
ATOM	73	CB	VAL	676	8.821	11.336	20.153	1.00	36.30	C
ATOM	74	CG1	VAL	676	7.421	11.860	20.358	1.00	29.55	C
ATOM	75	CG2	VAL	676	9.187	10.341	21.236	1.00	30.15	C
ATOM	76	C	VAL	676	8.669	11.777	17.736	1.00	39.08	C
ATOM	77	O	VAL	676	7.631	11.798	17.072	1.00	43.18	O
ATOM	78	N	LEU	677	9.637	12.667	17.547	1.00	38.08	N
ATOM	80	CA	LEU	677	9.429	13.726	16.565	1.00	37.80	C
ATOM	81	CB	LEU	677	10.571	14.726	16.574	1.00	34.97	C
ATOM	82	CG	LEU	677	10.812	15.352	17.943	1.00	40.42	C
ATOM	83	CD1	LEU	677	11.862	16.404	17.760	1.00	35.87	C
ATOM	84	CD2	LEU	677	9.511	15.944	18.534	1.00	39.49	C
ATOM	85	C	LEU	677	9.188	13.208	15.156	1.00	38.78	C
ATOM	86	O	LEU	677	8.324	13.730	14.448	1.00	44.11	O
ATOM	87	N	GLU	678	9.927	12.170	14.764	1.00	34.27	N
ATOM	89	CA	GLU	678	9.788	11.576	13.433	1.00	33.68	C
ATOM	90	CB	GLU	678	10.972	10.692	13.139	1.00	41.54	C
ATOM	91	CG	GLU	678	12.250	11.475	13.231	1.00	62.50	C
ATOM	92	CD	GLU	678	13.492	10.632	13.140	1.00	75.90	C
ATOM	93	OE1	GLU	678	14.581	11.222	12.946	1.00	77.79	O
ATOM	94	OE2	GLU	678	13.382	9.393	13.275	1.00	81.73	O
ATOM	95	C	GLU	678	8.502	10.791	13.361	1.00	31.24	C
ATOM	96	O	GLU	678	7.837	10.730	12.318	1.00	29.04	O
ATOM	97	N	ALA	679	8.118	10.229	14.496	1.00	27.29	N
ATOM	99	CA	ALA	679	6.878	9.486	14.561	1.00	31.51	C
ATOM	100	CB	ALA	679	6.807	8.699	15.862	1.00	32.16	C
ATOM	101	C	ALA	679	5.658	10.400	14.416	1.00	37.88	C
ATOM	102	O	ALA	679	4.657	10.013	13.784	1.00	39.80	O
ATOM	103	N	ILE	680	5.748	11.621	14.958	1.00	36.75	N
ATOM	105	CA	ILE	680	4.623	12.567	14.893	1.00	33.51	C
ATOM	106	CB	ILE	680	4.445	13.322	16.204	1.00	36.86	C
ATOM	107	CG2	ILE	680	4.222	12.324	17.343	1.00	34.87	C
ATOM	108	CG1	ILE	680	5.672	14.178	16.493	1.00	39.01	C
ATOM	109	CD1	ILE	680	5.503	15.046	17.719	1.00	38.54	C
ATOM	110	C	ILE	680	4.603	13.553	13.732	1.00	29.78	C
ATOM	111	O	ILE	680	3.560	14.137	13.425	1.00	35.01	O
ATOM	112	N	GLU	681	5.732	13.677	13.044	1.00	31.29	N
ATOM	114	CA	GLU	681	5.833	14.570	11.904	1.00	36.50	C
ATOM	115	CB	GLU	681	7.101	14.285	11.106	1.00	33.49	C
ATOM	116	CG	GLU	681	7.361	15.322	10.028	1.00	41.42	C
ATOM	117	CD	GLU	681	7.500	16.742	10.581	1.00	49.46	C
ATOM	118	OE1	GLU	681	7.569	16.924	11.824	1.00	44.22	O
ATOM	119	OE2	GLU	681	7.527	17.687	9.759	1.00	52.12	O
ATOM	120	C	GLU	681	4.638	14.373	11.013	1.00	38.74	C
ATOM	121	O	GLU	681	4.348	13.251	10.596	1.00	46.06	O
ATOM	122	N	PRO	682	3.892	15.446	10.751	1.00	41.06	N
ATOM	123	CD	PRO	682	4.159	16.800	11.261	1.00	39.59	C
ATOM	124	CA	PRO	682	2.695	15.422	9.904	1.00	41.12	C
ATOM	125	CB	PRO	682	2.214	16.870	9.965	1.00	43.30	C
ATOM	126	CG	PRO	682	2.800	17.399	11.250	1.00	38.89	C
ATOM	127	C	PRO	682	2.968	14.980	8.444	1.00	44.28	C

FIG. 6 CONT'D

ATOM	128	O	PRO	682	4.076	15.133	7.920	1.00 36.92	O
ATOM	129	N	GLY	683	1.943	14.446	7.788	1.00 48.21	N
ATOM	131	CA	GLY	683	2.103	13.990	6.416	1.00 51.13	C
ATOM	132	C	GLY	683	1.905	15.043	5.334	1.00 54.68	C
ATOM	133	O	GLY	683	1.817	16.226	5.629	1.00 63.53	O
ATOM	134	N	VAL	684	1.729	14.601	4.089	1.00 57.20	N
ATOM	136	CA	VAL	684	1.544	15.505	2.959	1.00 54.91	C
ATOM	137	CB	VAL	684	1.805	14.792	1.625	1.00 51.72	C
ATOM	138	CG1	VAL	684	1.618	15.769	0.487	1.00 53.17	C
ATOM	139	CG2	VAL	684	3.222	14.212	1.591	1.00 53.92	C
ATOM	140	C	VAL	684	0.123	16.048	2.952	1.00 54.45	C
ATOM	141	O	VAL	684	-0.828	15.287	2.775	1.00 57.51	O
ATOM	142	N	VAL	685	-0.021	17.360	3.125	1.00 48.43	N
ATOM	144	CA	VAL	685	-1.341	17.974	3.163	1.00 44.96	C
ATOM	145	CB	VAL	685	-1.455	18.932	4.355	1.00 39.06	C
ATOM	146	CG1	VAL	685	-2.888	19.062	4.764	1.00 41.14	C
ATOM	147	CG2	VAL	685	-0.611	18.445	5.520	1.00 36.12	C
ATOM	148	C	VAL	685	-1.603	18.758	1.887	1.00 46.69	C
ATOM	149	O	VAL	685	-0.934	19.742	1.644	1.00 54.09	O
ATOM	150	N	CYS	686	-2.582	18.340	1.087	1.00 51.49	N
ATOM	152	CA	CYS	686	-2.921	19.015	-0.177	1.00 55.13	C
ATOM	153	CB	CYS	686	-3.559	18.009	-1.155	1.00 57.05	C
ATOM	154	SG	CYS	686	-2.391	16.910	-2.025	1.00 65.52	S
ATOM	155	C	CYS	686	-3.830	20.266	-0.010	1.00 56.12	C
ATOM	156	O	CYS	686	-4.856	20.208	0.681	1.00 54.29	O
ATOM	157	N	ALA	687	-3.484	21.374	-0.681	1.00 54.36	N
ATOM	159	CA	ALA	687	-4.248	22.631	-0.584	1.00 54.20	C
ATOM	160	CB	ALA	687	-3.463	23.815	-1.168	1.00 49.21	C
ATOM	161	C	ALA	687	-5.583	22.542	-1.268	1.00 60.58	C
ATOM	162	O	ALA	687	-6.557	23.131	-0.803	1.00 62.87	O
ATOM	163	N	GLY	688	-5.623	21.791	-2.366	1.00 67.12	N
ATOM	165	CA	GLY	688	-6.847	21.650	-3.134	1.00 66.26	C
ATOM	166	C	GLY	688	-6.948	22.874	-4.024	1.00 64.95	C
ATOM	167	O	GLY	688	-7.888	23.676	-3.924	1.00 66.95	O
ATOM	168	N	HIS	689	-5.951	23.042	-4.879	1.00 59.22	N
ATOM	170	CA	HIS	689	-5.925	24.179	-5.769	1.00 54.36	C
ATOM	171	CB	HIS	689	-4.650	24.977	-5.537	1.00 46.90	C
ATOM	172	CG	HIS	689	-4.364	25.964	-6.617	1.00 52.16	C
ATOM	173	CD2	HIS	689	-3.474	25.931	-7.633	1.00 58.89	C
ATOM	174	ND1	HIS	689	-5.104	27.116	-6.787	1.00 52.66	N
ATOM	176	CE1	HIS	689	-4.683	27.750	-7.868	1.00 57.16	C
ATOM	177	NE2	HIS	689	-3.695	27.052	-8.402	1.00 60.29	N
ATOM	179	C	HIS	689	-6.022	23.716	-7.220	1.00 59.75	C
ATOM	180	O	HIS	689	-5.393	22.717	-7.602	1.00 62.11	O
ATOM	181	N	ASP	690	-6.838	24.424	-8.011	1.00 60.46	N
ATOM	183	CA	ASP	690	-7.021	24.108	-9.427	1.00 59.31	C
ATOM	184	CB	ASP	690	-8.334	24.701	-9.949	1.00 60.31	C
ATOM	185	CG	ASP	690	-8.762	24.107	-11.304	1.00 62.54	C
ATOM	186	OD1	ASP	690	-7.904	23.586	-12.054	1.00 54.14	O
ATOM	187	OD2	ASP	690	-9.970	24.166	-11.620	1.00 59.85	O
ATOM	188	C	ASP	690	-5.835	24.583	-10.280	1.00 60.15	C
ATOM	189	O	ASP	690	-5.739	25.752	-10.654	1.00 58.71	O
ATOM	190	N	ASN	691	-4.925	23.657	-10.564	1.00 66.30	N
ATOM	192	CA	ASN	691	-3.736	23.940	-11.369	1.00 71.61	C
ATOM	193	CB	ASN	691	-2.581	22.971	-11.016	1.00 72.66	C
ATOM	194	CG	ASN	691	-1.672	23.506	-9.923	1.00 72.16	C

FIG. 6 CONT'D

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ATOM    195  OD1 ASN   691      -1.697  24.697  -9.600  1.00 74.90      O
ATOM    196  ND2 ASN   691      -0.845  22.633  -9.365  1.00 72.55      N
ATOM    199  C   ASN   691      -4.037  23.857 -12.868  1.00 73.70      C
ATOM    200  O   ASN   691      -3.121  23.715 -13.682  1.00 81.27      O
ATOM    201  N   ASN   692      -5.317  23.908 -13.227  1.00 70.75      N
ATOM    203  CA  ASN   692      -5.705  23.851 -14.632  1.00 69.77      C
ATOM    204  CB  ASN   692      -6.551  22.600 -14.958  1.00 68.43      C
ATOM    205  CG  ASN   692      -6.019  21.331 -14.307  1.00 63.97      C
ATOM    206  OD1 ASN   692      -5.501  20.438 -14.972  0.00 65.30      O
ATOM    207  ND2 ASN   692      -6.184  21.240 -12.993  0.00 65.24      N
ATOM    210  C   ASN   692      -6.467  25.131 -14.982  1.00 66.04      C
ATOM    211  O   ASN   692      -6.986  25.257 -16.087  1.00 65.61      O
ATOM    212  N   GLN   693      -6.597  26.035 -14.005  1.00 67.69      N
ATOM    214  CA  GLN   693      -7.255  27.340 -14.196  1.00 71.99      C
ATOM    215  CB  GLN   693      -8.279  27.647 -13.084  1.00 68.47      C
ATOM    216  CG  GLN   693      -9.575  26.819 -13.134  1.00 72.04      C
ATOM    217  CD  GLN   693     -10.172  26.661 -14.540  1.00 75.91      C
ATOM    218  OE1 GLN   693      -9.955  27.497 -15.423  1.00 85.37      O
ATOM    219  NE2 GLN   693     -10.936  25.592 -14.745  1.00 70.58      N
ATOM    222  C   GLN   693      -6.171  28.429 -14.199  1.00 74.61      C
ATOM    223  O   GLN   693      -5.230  28.359 -13.413  1.00 73.58      O
ATOM    224  N   PRO   694      -6.285  29.438 -15.091  1.00 81.70      N
ATOM    225  CD  PRO   694      -7.398  29.662 -16.034  1.00 87.17      C
ATOM    226  CA  PRO   694      -5.302  30.531 -15.181  1.00 80.62      C
ATOM    227  CB  PRO   694      -5.911  31.458 -16.243  1.00 85.84      C
ATOM    228  CG  PRO   694      -7.421  31.170 -16.151  1.00 89.04      C
ATOM    229  C   PRO   694      -5.118  31.249 -13.856  1.00 77.25      C
ATOM    230  O   PRO   694      -6.106  31.640 -13.206  1.00 74.33      O
ATOM    231  N   ASP   695      -3.849  31.467 -13.496  1.00 76.00      N
ATOM    233  CA  ASP   695      -3.494  32.117 -12.237  1.00 63.22      C
ATOM    234  CB  ASP   695      -1.995  32.405 -12.153  1.00 63.70      C
ATOM    235  CG  ASP   695      -1.190  31.192 -11.684  1.00 66.50      C
ATOM    236  OD1 ASP   695      -1.523  30.627 -10.617  1.00 66.69      O
ATOM    237  OD2 ASP   695      -0.217  30.802 -12.377  1.00 71.13      O
ATOM    238  C   ASP   695      -4.294  33.356 -11.942  1.00 56.02      C
ATOM    239  O   ASP   695      -4.859  33.997 -12.842  1.00 56.35      O
ATOM    240  N   SER   696      -4.338  33.694 -10.666  1.00 56.40      N
ATOM    242  CA  SER   696      -5.093  34.839 -10.214  1.00 56.56      C
ATOM    243  CB  SER   696      -6.587  34.510 -10.289  1.00 54.32      C
ATOM    244  OG  SER   696      -7.365  35.473  -9.604  1.00 54.41      O
ATOM    246  C   SER   696      -4.690  35.191  -8.788  1.00 61.68      C
ATOM    247  O   SER   696      -4.326  34.319  -7.993  1.00 69.36      O
ATOM    248  N   PHE   697      -4.754  36.477  -8.474  1.00 61.93      N
ATOM    250  CA  PHE   697      -4.412  36.974  -7.153  1.00 61.05      C
ATOM    251  CB  PHE   697      -4.413  38.509  -7.195  1.00 63.27      C
ATOM    252  CG  PHE   697      -4.961  39.156  -5.951  1.00 60.53      C
ATOM    253  CD1 PHE   697      -4.142  39.397  -4.856  1.00 65.55      C
ATOM    254  CD2 PHE   697      -6.306  39.484  -5.864  1.00 61.74      C
ATOM    255  CE1 PHE   697      -4.651  39.950  -3.691  1.00 63.81      C
ATOM    256  CE2 PHE   697      -6.825  40.034  -4.710  1.00 66.91      C
ATOM    257  CZ  PHE   697      -5.994  40.267  -3.617  1.00 69.41      C
ATOM    258  C   PHE   697      -5.344  36.448  -6.037  1.00 61.34      C
ATOM    259  O   PHE   697      -4.881  36.053  -4.971  1.00 62.55      O
ATOM    260  N   ALA   698      -6.653  36.464  -6.261  1.00 58.96      N
ATOM    262  CA  ALA   698      -7.577  35.996  -5.230  1.00 59.58      C
ATOM    263  CB  ALA   698      -8.965  36.589  -5.448  1.00 56.65      C
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FIG. 6 CONT'D

ATOM	264	C	ALA	698	-7.653	34.467	-5.143	1.00 61.20	C
ATOM	265	O	ALA	698	-7.862	33.913	-4.063	1.00 64.62	O
ATOM	266	N	ALA	699	-7.492	33.783	-6.272	1.00 58.65	N
ATOM	268	CA	ALA	699	-7.555	32.328	-6.270	1.00 57.39	C
ATOM	269	CB	ALA	699	-7.749	31.791	-7.694	1.00 58.30	C
ATOM	270	C	ALA	699	-6.290	31.748	-5.616	1.00 54.55	C
ATOM	271	O	ALA	699	-6.349	30.708	-4.951	1.00 57.04	O
ATOM	272	N	LEU	700	-5.155	32.423	-5.786	1.00 44.77	N
ATOM	274	CA	LEU	700	-3.921	31.956	-5.181	1.00 40.04	C
ATOM	275	CB	LEU	700	-2.709	32.661	-5.800	1.00 40.84	C
ATOM	276	CG	LEU	700	-2.369	32.286	-7.251	1.00 47.93	C
ATOM	277	CD1	LEU	700	-1.195	33.092	-7.751	1.00 52.49	C
ATOM	278	CD2	LEU	700	-2.035	30.824	-7.337	1.00 41.70	C
ATOM	279	C	LEU	700	-3.983	32.180	-3.667	1.00 40.02	C
ATOM	280	O	LEU	700	-3.737	31.256	-2.893	1.00 42.09	O
ATOM	281	N	LEU	701	-4.384	33.375	-3.238	1.00 38.79	N
ATOM	283	CA	LEU	701	-4.468	33.679	-1.808	1.00 40.37	C
ATOM	284	CB	LEU	701	-4.545	35.190	-1.561	1.00 37.85	C
ATOM	285	CG	LEU	701	-3.253	35.971	-1.868	1.00 41.30	C
ATOM	286	CD1	LEU	701	-3.479	37.426	-1.612	1.00 41.50	C
ATOM	287	CD2	LEU	701	-2.070	35.506	-1.025	1.00 35.31	C
ATOM	288	C	LEU	701	-5.548	32.917	-1.024	1.00 45.30	C
ATOM	289	O	LEU	701	-5.305	32.557	0.128	1.00 45.13	O
ATOM	290	N	SER	702	-6.719	32.678	-1.633	1.00 52.36	N
ATOM	292	CA	SER	702	-7.822	31.899	-1.013	1.00 54.37	C
ATOM	293	CB	SER	702	-9.060	31.920	-1.914	1.00 50.95	C
ATOM	294	OG	SER	702	-9.500	33.246	-2.101	1.00 50.66	O
ATOM	296	C	SER	702	-7.388	30.433	-0.783	1.00 51.62	C
ATOM	297	O	SER	702	-7.740	29.806	0.234	1.00 45.03	O
ATOM	298	N	SER	703	-6.649	29.890	-1.756	1.00 49.24	N
ATOM	300	CA	SER	703	-6.119	28.536	-1.660	1.00 46.51	C
ATOM	301	CB	SER	703	-5.442	28.115	-2.956	1.00 37.23	C
ATOM	302	OG	SER	703	-6.388	28.080	-4.005	1.00 45.32	O
ATOM	304	C	SER	703	-5.101	28.504	-0.528	1.00 46.34	C
ATOM	305	O	SER	703	-5.141	27.597	0.293	1.00 52.79	O
ATOM	306	N	LEU	704	-4.215	29.501	-0.459	1.00 40.74	N
ATOM	308	CA	LEU	704	-3.227	29.548	0.618	1.00 36.98	C
ATOM	309	CB	LEU	704	-2.302	30.751	0.485	1.00 30.44	C
ATOM	310	CG	LEU	704	-0.994	30.563	-0.291	1.00 35.89	C
ATOM	311	CD1	LEU	704	-0.235	31.859	-0.308	1.00 36.89	C
ATOM	312	CD2	LEU	704	-0.115	29.484	0.307	1.00 37.91	C
ATOM	313	C	LEU	704	-3.902	29.552	1.984	1.00 41.66	C
ATOM	314	O	LEU	704	-3.389	28.951	2.920	1.00 45.02	O
ATOM	315	N	ASN	705	-5.061	30.208	2.076	1.00 45.16	N
ATOM	317	CA	ASN	705	-5.849	30.289	3.311	1.00 43.35	C
ATOM	318	CB	ASN	705	-6.934	31.370	3.201	1.00 44.83	C
ATOM	319	CG	ASN	705	-6.362	32.771	3.137	1.00 43.71	C
ATOM	320	OD1	ASN	705	-5.197	32.992	3.470	1.00 48.81	O
ATOM	321	ND2	ASN	705	-7.176	33.726	2.694	1.00 38.59	N
ATOM	324	C	ASN	705	-6.521	28.962	3.618	1.00 42.54	C
ATOM	325	O	ASN	705	-6.677	28.594	4.779	1.00 40.34	O
ATOM	326	N	GLU	706	-6.991	28.269	2.591	1.00 42.62	N
ATOM	328	CA	GLU	706	-7.607	26.987	2.842	1.00 44.02	C
ATOM	329	CB	GLU	706	-8.352	26.472	1.621	1.00 45.19	C
ATOM	330	CG	GLU	706	-9.322	25.338	1.971	1.00 55.97	C
ATOM	331	CD	GLU	706	-10.417	25.735	2.986	1.00 58.77	C

FIG. 6 CONT'D

ATOM	332	OE1	GLU	706	-10.707	24.945	3.918	1.00 60.16	O
ATOM	333	OE2	GLU	706	-11.019	26.817	2.838	1.00 60.87	O
ATOM	334	C	GLU	706	-6.478	26.033	3.261	1.00 42.46	C
ATOM	335	O	GLU	706	-6.639	25.253	4.195	1.00 42.70	O
ATOM	336	N	LEU	707	-5.307	26.167	2.636	1.00 38.31	N
ATOM	338	CA	LEU	707	-4.152	25.342	2.982	1.00 37.96	C
ATOM	339	CB	LEU	707	-2.958	25.608	2.046	1.00 35.41	C
ATOM	340	CG	LEU	707	-1.651	24.872	2.392	1.00 35.71	C
ATOM	341	CD1	LEU	707	-1.895	23.385	2.326	1.00 38.82	C
ATOM	342	CD2	LEU	707	-0.518	25.239	1.459	1.00 33.25	C
ATOM	343	C	LEU	707	-3.767	25.654	4.431	1.00 44.27	C
ATOM	344	O	LEU	707	-3.464	24.747	5.211	1.00 51.41	O
ATOM	345	N	GLY	708	-3.782	26.938	4.787	1.00 45.88	N
ATOM	347	CA	GLY	708	-3.463	27.344	6.144	1.00 40.92	C
ATOM	348	C	GLY	708	-4.386	26.618	7.096	1.00 39.05	C
ATOM	349	O	GLY	708	-3.937	25.851	7.924	1.00 45.81	O
ATOM	350	N	GLU	709	-5.685	26.790	6.913	1.00 46.04	N
ATOM	352	CA	GLU	709	-6.680	26.125	7.758	1.00 51.25	C
ATOM	353	CB	GLU	709	-8.079	26.273	7.151	1.00 56.56	C
ATOM	354	CG	GLU	709	-9.198	25.652	7.984	1.00 63.02	C
ATOM	355	CD	GLU	709	-9.766	26.593	9.042	1.00 64.61	C
ATOM	356	OE1	GLU	709	-10.855	26.293	9.573	1.00 65.41	O
ATOM	357	OE2	GLU	709	-9.157	27.641	9.338	1.00 66.14	O
ATOM	358	C	GLU	709	-6.367	24.637	7.975	1.00 51.93	C
ATOM	359	O	GLU	709	-6.213	24.197	9.107	1.00 56.39	O
ATOM	360	N	ARG	710	-6.235	23.864	6.901	1.00 53.43	N
ATOM	362	CA	ARG	710	-5.938	22.440	7.058	1.00 50.19	C
ATOM	363	CB	ARG	710	-6.032	21.652	5.747	1.00 56.69	C
ATOM	364	CG	ARG	710	-6.192	22.446	4.493	1.00 59.66	C
ATOM	365	CD	ARG	710	-7.462	22.035	3.786	1.00 59.37	C
ATOM	366	NE	ARG	710	-7.203	21.172	2.643	1.00 58.69	N
ATOM	368	CZ	ARG	710	-8.124	20.857	1.736	1.00 70.01	C
ATOM	369	NH1	ARG	710	-9.364	21.349	1.854	1.00 75.20	N
ATOM	372	NH2	ARG	710	-7.812	20.057	0.713	1.00 65.26	N
ATOM	375	C	ARG	710	-4.617	22.102	7.735	1.00 44.91	C
ATOM	376	O	ARG	710	-4.522	21.061	8.396	1.00 43.38	O
ATOM	377	N	GLN	711	-3.596	22.939	7.556	1.00 40.11	N
ATOM	379	CA	GLN	711	-2.310	22.685	8.189	1.00 34.69	C
ATOM	380	CB	GLN	711	-1.194	23.478	7.542	1.00 42.15	C
ATOM	381	CG	GLN	711	-0.753	22.877	6.244	1.00 43.03	C
ATOM	382	CD	GLN	711	0.553	23.442	5.779	1.00 44.24	C
ATOM	383	OE1	GLN	711	1.321	23.988	6.567	1.00 54.32	O
ATOM	384	NE2	GLN	711	0.828	23.305	4.496	1.00 52.33	N
ATOM	387	C	GLN	711	-2.355	23.007	9.653	1.00 36.60	C
ATOM	388	O	GLN	711	-1.501	22.557	10.408	1.00 40.79	O
ATOM	389	N	LEU	712	-3.361	23.778	10.054	1.00 41.25	N
ATOM	391	CA	LEU	712	-3.561	24.163	11.457	1.00 43.47	C
ATOM	392	CB	LEU	712	-4.585	25.295	11.550	1.00 42.08	C
ATOM	393	CG	LEU	712	-4.829	25.943	12.905	1.00 45.04	C
ATOM	394	CD1	LEU	712	-3.489	26.199	13.594	1.00 48.18	C
ATOM	395	CD2	LEU	712	-5.610	27.248	12.711	1.00 44.32	C
ATOM	396	C	LEU	712	-4.061	22.938	12.222	1.00 45.20	C
ATOM	397	O	LEU	712	-3.595	22.628	13.320	1.00 46.51	O
ATOM	398	N	VAL	713	-5.014	22.240	11.623	1.00 42.76	N
ATOM	400	CA	VAL	713	-5.555	21.026	12.198	1.00 41.99	C
ATOM	401	CB	VAL	713	-6.480	20.348	11.170	1.00 43.85	C

FIG. 6 CONT'D

ATOM	402	CG1	VAL	713	-6.887	18.953	11.628	1.00 52.59	C
ATOM	403	CG2	VAL	713	-7.708	21.203	10.966	1.00 42.38	C
ATOM	404	C	VAL	713	-4.383	20.100	12.562	1.00 45.10	C
ATOM	405	O	VAL	713	-4.275	19.646	13.703	1.00 45.64	O
ATOM	406	N	HIS	714	-3.471	19.905	11.604	1.00 46.35	N
ATOM	408	CA	HIS	714	-2.286	19.044	11.767	1.00 45.95	C
ATOM	409	CB	HIS	714	-1.458	18.971	10.487	1.00 49.61	C
ATOM	410	CG	HIS	714	-1.950	17.947	9.519	1.00 62.09	C
ATOM	411	CD2	HIS	714	-1.404	16.778	9.108	1.00 64.82	C
ATOM	412	ND1	HIS	714	-3.157	18.058	8.873	1.00 63.02	N
ATOM	414	CE1	HIS	714	-3.340	17.005	8.100	1.00 70.96	C
ATOM	415	NE2	HIS	714	-2.291	16.211	8.219	1.00 70.54	N
ATOM	417	C	HIS	714	-1.379	19.495	12.857	1.00 43.82	C
ATOM	418	O	HIS	714	-0.798	18.674	13.571	1.00 48.61	O
ATOM	419	N	VAL	715	-1.172	20.803	12.898	1.00 40.29	N
ATOM	421	CA	VAL	715	-0.326	21.415	13.908	1.00 39.63	C
ATOM	422	CB	VAL	715	-0.101	22.918	13.620	1.00 38.77	C
ATOM	423	CG1	VAL	715	0.500	23.617	14.820	1.00 30.17	C
ATOM	424	CG2	VAL	715	0.857	23.048	12.463	1.00 40.69	C
ATOM	425	C	VAL	715	-0.962	21.201	15.273	1.00 36.62	C
ATOM	426	O	VAL	715	-0.266	20.874	16.244	1.00 30.18	O
ATOM	427	N	VAL	716	-2.286	21.329	15.331	1.00 28.64	N
ATOM	429	CA	VAL	716	-2.994	21.113	16.570	1.00 28.84	C
ATOM	430	CB	VAL	716	-4.508	21.331	16.403	1.00 34.61	C
ATOM	431	CG1	VAL	716	-5.239	20.839	17.647	1.00 29.84	C
ATOM	432	CG2	VAL	716	-4.805	22.811	16.185	1.00 32.32	C
ATOM	433	C	VAL	716	-2.687	19.683	17.037	1.00 36.83	C
ATOM	434	O	VAL	716	-2.078	19.485	18.092	1.00 36.70	O
ATOM	435	N	LYS	717	-2.972	18.709	16.179	1.00 38.71	N
ATOM	437	CA	LYS	717	-2.737	17.313	16.505	1.00 32.14	C
ATOM	438	CB	LYS	717	-3.370	16.410	15.450	1.00 32.30	C
ATOM	439	CG	LYS	717	-4.890	16.352	15.569	1.00 38.88	C
ATOM	440	CD	LYS	717	-5.538	15.584	14.436	0.00 36.05	C
ATOM	441	CE	LYS	717	-7.009	15.353	14.736	0.00 36.14	C
ATOM	442	NZ	LYS	717	-7.739	14.704	13.619	0.00 35.32	N
ATOM	446	C	LYS	717	-1.263	16.990	16.699	1.00 32.82	C
ATOM	447	O	LYS	717	-0.920	16.262	17.631	1.00 34.86	O
ATOM	448	N	TRP	718	-0.383	17.589	15.893	1.00 31.69	N
ATOM	450	CA	TRP	718	1.058	17.319	16.010	1.00 34.84	C
ATOM	451	CB	TRP	718	1.850	17.995	14.883	1.00 25.87	C
ATOM	452	CG	TRP	718	3.343	18.092	15.136	1.00 25.59	C
ATOM	453	CD2	TRP	718	4.055	19.232	15.641	1.00 30.45	C
ATOM	454	CE2	TRP	718	5.419	18.889	15.689	1.00 30.51	C
ATOM	455	CE3	TRP	718	3.672	20.519	16.046	1.00 32.20	C
ATOM	456	CD1	TRP	718	4.279	17.133	14.909	1.00 35.87	C
ATOM	457	NE1	TRP	718	5.533	17.598	15.237	1.00 32.13	N
ATOM	459	CZ2	TRP	718	6.403	19.782	16.119	1.00 32.90	C
ATOM	460	CZ3	TRP	718	4.650	21.408	16.468	1.00 25.41	C
ATOM	461	CH2	TRP	718	5.997	21.036	16.503	1.00 28.69	C
ATOM	462	C	TRP	718	1.604	17.753	17.367	1.00 44.15	C
ATOM	463	O	TRP	718	2.347	17.014	18.020	1.00 48.94	O
ATOM	464	N	ALA	719	1.242	18.973	17.764	1.00 56.34	N
ATOM	466	CA	ALA	719	1.654	19.580	19.037	1.00 52.43	C
ATOM	467	CB	ALA	719	1.214	21.043	19.073	1.00 48.46	C
ATOM	468	C	ALA	719	1.176	18.846	20.305	1.00 47.73	C
ATOM	469	O	ALA	719	1.968	18.662	21.246	1.00 46.60	O

FIG. 6 CONT'D

ATOM	470	N	LYS	720	-0.107	18.461	20.337	1.00 42.77	N
ATOM	472	CA	LYS	720	-0.697	17.744	21.478	1.00 45.06	C
ATOM	473	CB	LYS	720	-2.218	17.567	21.294	1.00 39.13	C
ATOM	474	CG	LYS	720	-3.057	18.632	21.979	1.00 45.90	C
ATOM	475	CD	LYS	720	-4.533	18.253	22.075	1.00 55.06	C
ATOM	476	CE	LYS	720	-5.236	19.088	23.161	1.00 63.65	C
ATOM	477	NZ	LYS	720	-6.668	18.719	23.402	1.00 62.72	N
ATOM	481	C	LYS	720	-0.019	16.386	21.772	1.00 47.46	C
ATOM	482	O	LYS	720	-0.227	15.789	22.835	1.00 50.10	O
ATOM	483	N	ALA	721	0.810	15.926	20.842	1.00 40.80	N
ATOM	485	CA	ALA	721	1.524	14.671	20.995	1.00 41.77	C
ATOM	486	CB	ALA	721	1.410	13.840	19.710	1.00 45.25	C
ATOM	487	C	ALA	721	2.991	14.884	21.346	1.00 41.79	C
ATOM	488	O	ALA	721	3.762	13.931	21.370	1.00 43.57	O
ATOM	489	N	LEU	722	3.382	16.131	21.585	1.00 40.71	N
ATOM	491	CA	LEU	722	4.764	16.438	21.927	1.00 34.69	C
ATOM	492	CB	LEU	722	5.058	17.911	21.665	1.00 32.26	C
ATOM	493	CG	LEU	722	5.357	18.244	20.218	1.00 33.93	C
ATOM	494	CD1	LEU	722	5.226	19.728	20.021	1.00 43.98	C
ATOM	495	CD2	LEU	722	6.753	17.784	19.880	1.00 30.81	C
ATOM	496	C	LEU	722	5.115	16.085	23.369	1.00 33.82	C
ATOM	497	O	LEU	722	4.301	16.249	24.281	1.00 34.39	O
ATOM	498	N	PRO	723	6.338	15.589	23.592	1.00 37.66	N
ATOM	499	CD	PRO	723	7.354	15.282	22.562	1.00 41.22	C
ATOM	500	CA	PRO	723	6.820	15.209	24.917	1.00 35.69	C
ATOM	501	CB	PRO	723	8.285	14.855	24.662	1.00 34.40	C
ATOM	502	CG	PRO	723	8.272	14.339	23.283	1.00 36.44	C
ATOM	503	C	PRO	723	6.724	16.368	25.893	1.00 39.06	C
ATOM	504	O	PRO	723	7.512	17.304	25.833	1.00 39.26	O
ATOM	505	N	GLY	724	5.780	16.284	26.812	1.00 39.75	N
ATOM	507	CA	GLY	724	5.652	17.336	27.794	1.00 34.24	C
ATOM	508	C	GLY	724	4.544	18.311	27.480	1.00 36.36	C
ATOM	509	O	GLY	724	3.911	18.837	28.398	1.00 37.90	O
ATOM	510	N	PHE	725	4.212	18.465	26.201	1.00 32.86	N
ATOM	512	CA	PHE	725	3.192	19.422	25.845	1.00 36.30	C
ATOM	513	CB	PHE	725	2.842	19.365	24.383	1.00 32.46	C
ATOM	514	CG	PHE	725	1.928	20.474	23.958	1.00 37.13	C
ATOM	515	CD1	PHE	725	2.453	21.687	23.542	1.00 37.70	C
ATOM	516	CD2	PHE	725	0.544	20.302	23.948	1.00 39.17	C
ATOM	517	CE1	PHE	725	1.618	22.717	23.107	1.00 36.54	C
ATOM	518	CE2	PHE	725	-0.308	21.331	23.513	1.00 39.69	C
ATOM	519	CZ	PHE	725	0.233	22.540	23.089	1.00 42.41	C
ATOM	520	C	PHE	725	1.899	19.385	26.620	1.00 41.59	C
ATOM	521	O	PHE	725	1.385	20.441	27.002	1.00 44.02	O
ATOM	522	N	ARG	726	1.335	18.189	26.791	1.00 49.80	N
ATOM	524	CA	ARG	726	0.050	18.042	27.489	1.00 49.46	C
ATOM	525	CB	ARG	726	-0.652	16.709	27.154	1.00 44.05	C
ATOM	526	CG	ARG	726	-1.692	16.821	26.023	1.00 44.55	C
ATOM	527	CD	ARG	726	-2.598	15.606	26.003	1.00 48.35	C
ATOM	528	NE	ARG	726	-3.771	15.752	25.130	1.00 56.42	N
ATOM	530	CZ	ARG	726	-5.040	15.569	25.526	1.00 62.91	C
ATOM	531	NH1	ARG	726	-5.323	15.249	26.799	1.00 55.81	N
ATOM	534	NH2	ARG	726	-6.028	15.649	24.632	1.00 55.35	N
ATOM	537	C	ARG	726	0.057	18.304	28.995	1.00 52.43	C
ATOM	538	O	ARG	726	-0.978	18.139	29.644	1.00 52.56	O
ATOM	539	N	ASN	727	1.213	18.685	29.551	1.00 53.84	N

FIG. 6 CONT'D

ATOM	541	CA	ASN	727	1.292	19.018	30.969	1.00	58.03	C
ATOM	542	CB	ASN	727	2.636	18.589	31.604	1.00	63.66	C
ATOM	543	CG	ASN	727	3.777	19.597	31.388	1.00	67.51	C
ATOM	544	OD1	ASN	727	4.837	19.234	30.881	1.00	68.14	O
ATOM	545	ND2	ASN	727	3.606	20.828	31.864	1.00	73.64	N
ATOM	548	C	ASN	727	1.026	20.528	31.138	1.00	61.72	C
ATOM	549	O	ASN	727	0.723	20.993	32.248	1.00	65.35	O
ATOM	550	N	LEU	728	1.190	21.288	30.047	1.00	59.72	N
ATOM	552	CA	LEU	728	0.957	22.739	30.035	1.00	50.93	C
ATOM	553	CB	LEU	728	1.369	23.348	28.695	1.00	54.70	C
ATOM	554	CG	LEU	728	2.822	23.408	28.228	1.00	52.07	C
ATOM	555	CD1	LEU	728	2.808	24.029	26.844	1.00	45.38	C
ATOM	556	CD2	LEU	728	3.700	24.223	29.181	1.00	47.21	C
ATOM	557	C	LEU	728	-0.520	23.033	30.227	1.00	47.17	C
ATOM	558	O	LEU	728	-1.365	22.247	29.822	1.00	45.55	O
ATOM	559	N	HIS	729	-0.841	24.201	30.763	1.00	45.54	N
ATOM	561	CA	HIS	729	-2.231	24.530	30.986	1.00	44.10	C
ATOM	562	CB	HIS	729	-2.328	25.851	31.716	1.00	54.55	C
ATOM	563	CG	HIS	729	-3.717	26.221	32.119	1.00	63.22	C
ATOM	564	CD2	HIS	729	-4.893	26.156	31.442	1.00	66.57	C
ATOM	565	ND1	HIS	729	-4.016	26.777	33.340	1.00	63.71	N
ATOM	567	CE1	HIS	729	-5.308	27.046	33.401	1.00	68.21	C
ATOM	568	NE2	HIS	729	-5.861	26.678	32.256	1.00	68.48	N
ATOM	570	C	HIS	729	-2.972	24.559	29.655	1.00	40.23	C
ATOM	571	O	HIS	729	-2.421	24.976	28.658	1.00	44.09	O
ATOM	572	N	VAL	730	-4.224	24.116	29.653	1.00	39.50	N
ATOM	574	CA	VAL	730	-5.024	24.042	28.433	1.00	42.50	C
ATOM	575	CB	VAL	730	-6.500	23.653	28.710	1.00	50.67	C
ATOM	576	CG1	VAL	730	-7.044	24.387	29.936	1.00	48.50	C
ATOM	577	CG2	VAL	730	-7.367	23.960	27.478	1.00	50.44	C
ATOM	578	C	VAL	730	-5.016	25.262	27.563	1.00	45.07	C
ATOM	579	O	VAL	730	-4.893	25.178	26.339	1.00	50.12	O
ATOM	580	N	ASP	731	-5.249	26.399	28.185	1.00	51.13	N
ATOM	582	CA	ASP	731	-5.269	27.646	27.453	1.00	51.89	C
ATOM	583	CB	ASP	731	-5.820	28.755	28.338	1.00	51.89	C
ATOM	584	CG	ASP	731	-7.194	28.415	28.872	1.00	59.37	C
ATOM	585	OD1	ASP	731	-8.065	28.082	28.030	1.00	56.09	O
ATOM	586	OD2	ASP	731	-7.373	28.414	30.122	1.00	61.65	O
ATOM	587	C	ASP	731	-3.856	27.909	26.971	1.00	46.10	C
ATOM	588	O	ASP	731	-3.663	28.213	25.810	1.00	51.50	O
ATOM	589	N	ASP	732	-2.862	27.675	27.814	1.00	37.19	N
ATOM	591	CA	ASP	732	-1.482	27.861	27.392	1.00	37.51	C
ATOM	592	CB	ASP	732	-0.516	27.597	28.536	1.00	40.29	C
ATOM	593	CG	ASP	732	-0.523	28.713	29.565	1.00	51.89	C
ATOM	594	OD1	ASP	732	-1.171	29.755	29.313	1.00	56.09	O
ATOM	595	OD2	ASP	732	0.116	28.562	30.631	1.00	59.50	O
ATOM	596	C	ASP	732	-1.177	26.934	26.232	1.00	39.98	C
ATOM	597	O	ASP	732	-0.398	27.268	25.351	1.00	44.52	O
ATOM	598	N	GLN	733	-1.819	25.776	26.213	1.00	46.01	N
ATOM	600	CA	GLN	733	-1.621	24.832	25.131	1.00	48.12	C
ATOM	601	CB	GLN	733	-2.421	23.563	25.364	1.00	52.94	C
ATOM	602	CG	GLN	733	-1.791	22.511	26.234	1.00	52.25	C
ATOM	603	CD	GLN	733	-2.659	21.287	26.227	1.00	53.92	C
ATOM	604	OE1	GLN	733	-3.252	20.925	27.238	1.00	59.82	O
ATOM	605	NE2	GLN	733	-2.836	20.701	25.051	1.00	55.07	N
ATOM	608	C	GLN	733	-2.183	25.485	23.884	1.00	48.61	C

FIG. 6 CONT'D

ATOM	609	O	GLN	733	-1.531	25.558	22.854	1.00 51.31	O
ATOM	610	N	MET	734	-3.416	25.952	23.993	1.00 48.02	N
ATOM	612	CA	MET	734	-4.107	26.588	22.887	1.00 50.74	C
ATOM	613	CB	MET	734	-5.545	26.832	23.297	1.00 56.63	C
ATOM	614	CG	MET	734	-6.530	26.884	22.158	1.00 71.95	C
ATOM	615	SD	MET	734	-8.226	26.806	22.797	1.00 94.18	S
ATOM	616	CE	MET	734	-7.929	26.442	24.662	1.00 83.04	C
ATOM	617	C	MET	734	-3.448	27.904	22.453	1.00 50.43	C
ATOM	618	O	MET	734	-3.495	28.269	21.286	1.00 53.47	O
ATOM	619	N	ALA	735	-2.779	28.577	23.384	1.00 49.75	N
ATOM	621	CA	ALA	735	-2.115	29.844	23.109	1.00 43.40	C
ATOM	622	CB	ALA	735	-1.845	30.602	24.406	1.00 36.08	C
ATOM	623	C	ALA	735	-0.820	29.686	22.305	1.00 43.42	C
ATOM	624	O	ALA	735	-0.749	30.185	21.185	1.00 51.41	O
ATOM	625	N	VAL	736	0.198	29.002	22.832	1.00 38.22	N
ATOM	627	CA	VAL	736	1.441	28.866	22.066	1.00 36.45	C
ATOM	628	CB	VAL	736	2.502	28.000	22.764	1.00 35.87	C
ATOM	629	CG1	VAL	736	3.048	28.714	23.978	1.00 44.32	C
ATOM	630	CG2	VAL	736	1.924	26.673	23.156	1.00 36.64	C
ATOM	631	C	VAL	736	1.210	28.345	20.651	1.00 36.01	C
ATOM	632	O	VAL	736	1.982	28.655	19.747	1.00 41.42	O
ATOM	633	N	ILE	737	0.132	27.585	20.465	1.00 30.08	N
ATOM	635	CA	ILE	737	-0.220	27.048	19.150	1.00 31.25	C
ATOM	636	CB	ILE	737	-1.361	25.992	19.250	1.00 32.49	C
ATOM	637	CG2	ILE	737	-2.061	25.803	17.907	1.00 22.38	C
ATOM	638	CG1	ILE	737	-0.781	24.654	19.749	1.00 36.28	C
ATOM	639	CD1	ILE	737	-1.792	23.707	20.422	1.00 39.52	C
ATOM	640	C	ILE	737	-0.623	28.195	18.241	1.00 32.22	C
ATOM	641	O	ILE	737	0.022	28.449	17.222	1.00 40.26	O
ATOM	642	N	GLN	738	-1.657	28.926	18.636	1.00 34.76	N
ATOM	644	CA	GLN	738	-2.127	30.064	17.857	1.00 36.96	C
ATOM	645	CB	GLN	738	-3.310	30.715	18.570	1.00 35.31	C
ATOM	646	CG	GLN	738	-4.548	29.817	18.615	1.00 36.30	C
ATOM	647	CD	GLN	738	-5.569	30.254	19.666	1.00 46.43	C
ATOM	648	OE1	GLN	738	-5.196	30.752	20.728	1.00 51.09	O
ATOM	649	NE2	GLN	738	-6.860	30.059	19.379	1.00 45.97	N
ATOM	652	C	GLN	738	-0.999	31.078	17.575	1.00 38.78	C
ATOM	653	O	GLN	738	-0.780	31.434	16.422	1.00 47.01	O
ATOM	654	N	TYR	739	-0.206	31.428	18.586	1.00 32.35	N
ATOM	656	CA	TYR	739	0.867	32.387	18.402	1.00 30.36	C
ATOM	657	CB	TYR	739	1.496	32.821	19.735	1.00 36.60	C
ATOM	658	CG	TYR	739	0.565	33.487	20.754	1.00 41.72	C
ATOM	659	CD1	TYR	739	0.736	33.272	22.126	1.00 44.87	C
ATOM	660	CE1	TYR	739	-0.163	33.808	23.073	1.00 39.98	C
ATOM	661	CD2	TYR	739	-0.515	34.267	20.358	1.00 43.18	C
ATOM	662	CE2	TYR	739	-1.416	34.803	21.303	1.00 43.31	C
ATOM	663	CZ	TYR	739	-1.239	34.561	22.649	1.00 38.00	C
ATOM	664	OH	TYR	739	-2.178	35.014	23.556	1.00 54.08	O
ATOM	666	C	TYR	739	1.975	31.867	17.526	1.00 34.27	C
ATOM	667	O	TYR	739	2.502	32.609	16.712	1.00 35.19	O
ATOM	668	N	SER	740	2.351	30.606	17.674	1.00 36.52	N
ATOM	670	CA	SER	740	3.459	30.114	16.875	1.00 38.17	C
ATOM	671	CB	SER	740	4.390	29.231	17.727	1.00 42.37	C
ATOM	672	OG	SER	740	3.756	28.053	18.200	1.00 39.05	O
ATOM	674	C	SER	740	3.129	29.453	15.535	1.00 38.14	C
ATOM	675	O	SER	740	4.024	29.259	14.706	1.00 41.67	O

FIG. 6 CONT'D

ATOM	676	N	TRP	741	1.851	29.268	15.236	1.00	32.00	N
ATOM	678	CA	TRP	741	1.482	28.588	14.004	1.00	32.79	C
ATOM	679	CB	TRP	741	-0.034	28.446	13.918	1.00	44.21	C
ATOM	680	CG	TRP	741	-0.733	29.487	13.136	1.00	58.12	C
ATOM	681	CD2	TRP	741	-1.365	29.303	11.870	1.00	63.13	C
ATOM	682	CE2	TRP	741	-1.882	30.562	11.473	1.00	67.95	C
ATOM	683	CE3	TRP	741	-1.558	28.194	11.031	1.00	57.71	C
ATOM	684	CD1	TRP	741	-0.889	30.806	13.458	1.00	64.16	C
ATOM	685	NE1	TRP	741	-1.574	31.462	12.462	1.00	67.31	N
ATOM	687	CZ2	TRP	741	-2.561	30.747	10.260	1.00	70.02	C
ATOM	688	CZ3	TRP	741	-2.232	28.373	9.831	1.00	59.16	C
ATOM	689	CH2	TRP	741	-2.731	29.642	9.458	1.00	65.30	C
ATOM	690	C	TRP	741	2.099	29.060	12.681	1.00	34.24	C
ATOM	691	O	TRP	741	2.578	28.250	11.891	1.00	34.43	O
ATOM	692	N	MET	742	2.184	30.370	12.489	1.00	41.58	N
ATOM	694	CA	MET	742	2.749	30.945	11.265	1.00	39.13	C
ATOM	695	CB	MET	742	2.689	32.476	11.309	1.00	42.39	C
ATOM	696	CG	MET	742	3.147	33.177	10.032	1.00	43.70	C
ATOM	697	SD	MET	742	1.988	32.993	8.658	1.00	45.17	S
ATOM	698	CE	MET	742	0.678	34.132	9.133	1.00	22.14	C
ATOM	699	C	MET	742	4.193	30.537	11.090	1.00	30.85	C
ATOM	700	O	MET	742	4.602	30.115	10.017	1.00	34.78	O
ATOM	701	N	GLY	743	4.954	30.648	12.165	1.00	24.94	N
ATOM	703	CA	GLY	743	6.367	30.312	12.117	1.00	27.24	C
ATOM	704	C	GLY	743	6.630	28.836	11.886	1.00	27.21	C
ATOM	705	O	GLY	743	7.660	28.461	11.322	1.00	27.69	O
ATOM	706	N	LEU	744	5.734	27.983	12.372	1.00	25.91	N
ATOM	708	CA	LEU	744	5.895	26.550	12.172	1.00	26.90	C
ATOM	709	CB	LEU	744	4.899	25.755	13.018	1.00	25.72	C
ATOM	710	CG	LEU	744	5.234	25.626	14.514	1.00	29.11	C
ATOM	711	CD1	LEU	744	4.063	25.022	15.275	1.00	23.25	C
ATOM	712	CD2	LEU	744	6.484	24.771	14.689	1.00	24.15	C
ATOM	713	C	LEU	744	5.632	26.287	10.708	1.00	27.04	C
ATOM	714	O	LEU	744	6.375	25.574	10.048	1.00	31.01	O
ATOM	715	N	MET	745	4.566	26.886	10.200	1.00	25.67	N
ATOM	717	CA	MET	745	4.188	26.725	8.803	1.00	23.96	C
ATOM	718	CB	MET	745	2.895	27.454	8.534	1.00	20.46	C
ATOM	719	CG	MET	745	1.730	26.888	9.310	1.00	19.98	C
ATOM	720	SD	MET	745	0.297	27.272	8.341	1.00	43.15	S
ATOM	721	CE	MET	745	0.642	29.041	8.042	1.00	44.27	C
ATOM	722	C	MET	745	5.254	27.179	7.822	1.00	29.61	C
ATOM	723	O	MET	745	5.550	26.480	6.857	1.00	34.60	O
ATOM	724	N	VAL	746	5.830	28.341	8.095	1.00	27.98	N
ATOM	726	CA	VAL	746	6.876	28.924	7.288	1.00	24.84	C
ATOM	727	CB	VAL	746	7.248	30.304	7.835	1.00	31.98	C
ATOM	728	CG1	VAL	746	8.423	30.888	7.073	1.00	29.03	C
ATOM	729	CG2	VAL	746	6.066	31.196	7.737	1.00	32.19	C
ATOM	730	C	VAL	746	8.107	28.051	7.345	1.00	28.42	C
ATOM	731	O	VAL	746	8.749	27.786	6.333	1.00	37.05	O
ATOM	732	N	PHE	747	8.439	27.607	8.541	1.00	31.29	N
ATOM	734	CA	PHE	747	9.605	26.765	8.736	1.00	32.19	C
ATOM	735	CB	PHE	747	9.820	26.536	10.224	1.00	27.90	C
ATOM	736	CG	PHE	747	11.209	26.082	10.573	1.00	26.00	C
ATOM	737	CD1	PHE	747	12.293	26.915	10.343	1.00	24.54	C
ATOM	738	CD2	PHE	747	11.428	24.846	11.166	1.00	27.23	C
ATOM	739	CE1	PHE	747	13.571	26.532	10.699	1.00	25.88	C

FIG. 6 CONT'D

ATOM	740	CE2	PHE	747	12.711	24.451	11.528	1.00 25.61	C
ATOM	741	CZ	PHE	747	13.785	25.297	11.293	1.00 28.75	C
ATOM	742	C	PHE	747	9.468	25.401	8.030	1.00 35.99	C
ATOM	743	O	PHE	747	10.398	24.916	7.384	1.00 34.95	O
ATOM	744	N	ALA	748	8.309	24.774	8.171	1.00 35.11	N
ATOM	746	CA	ALA	748	8.096	23.483	7.561	1.00 34.00	C
ATOM	747	CB	ALA	748	6.773	22.896	8.022	1.00 29.48	C
ATOM	748	C	ALA	748	8.114	23.683	6.054	1.00 37.26	C
ATOM	749	O	ALA	748	8.831	22.973	5.344	1.00 35.87	O
ATOM	750	N	MET	749	7.385	24.707	5.591	1.00 41.15	N
ATOM	752	CA	MET	749	7.277	25.044	4.167	1.00 33.31	C
ATOM	753	CB	MET	749	6.444	26.303	3.982	1.00 35.95	C
ATOM	754	CG	MET	749	6.179	26.682	2.542	1.00 45.47	C
ATOM	755	SD	MET	749	7.444	27.726	1.821	1.00 50.89	S
ATOM	756	CE	MET	749	7.553	28.954	3.104	1.00 55.72	C
ATOM	757	C	MET	749	8.647	25.225	3.563	1.00 35.12	C
ATOM	758	O	MET	749	8.934	24.711	2.491	1.00 37.94	O
ATOM	759	N	GLY	750	9.507	25.929	4.278	1.00 36.97	N
ATOM	761	CA	GLY	750	10.863	26.138	3.810	1.00 42.04	C
ATOM	762	C	GLY	750	11.628	24.828	3.715	1.00 43.22	C
ATOM	763	O	GLY	750	12.530	24.678	2.889	1.00 43.48	O
ATOM	764	N	TRP	751	11.304	23.876	4.581	1.00 45.43	N
ATOM	766	CA	TRP	751	11.976	22.588	4.528	1.00 42.53	C
ATOM	767	CB	TRP	751	11.717	21.776	5.787	1.00 39.21	C
ATOM	768	CG	TRP	751	12.359	20.401	5.737	1.00 41.85	C
ATOM	769	CD2	TRP	751	13.743	20.085	5.968	1.00 37.37	C
ATOM	770	CE2	TRP	751	13.878	18.692	5.821	1.00 41.26	C
ATOM	771	CE3	TRP	751	14.877	20.841	6.275	1.00 41.35	C
ATOM	772	CD1	TRP	751	11.736	19.213	5.461	1.00 39.44	C
ATOM	773	NE1	TRP	751	12.645	18.186	5.516	1.00 42.23	N
ATOM	775	CZ2	TRP	751	15.110	18.046	5.978	1.00 48.39	C
ATOM	776	CZ3	TRP	751	16.104	20.195	6.431	1.00 39.62	C
ATOM	777	CH2	TRP	751	16.208	18.817	6.280	1.00 43.38	C
ATOM	778	C	TRP	751	11.519	21.806	3.294	1.00 43.17	C
ATOM	779	O	TRP	751	12.336	21.207	2.596	1.00 40.24	O
ATOM	780	N	ARG	752	10.214	21.792	3.037	1.00 42.27	N
ATOM	782	CA	ARG	752	9.683	21.100	1.862	1.00 41.53	C
ATOM	783	CB	ARG	752	8.163	21.186	1.800	1.00 42.14	C
ATOM	784	CG	ARG	752	7.441	20.465	2.920	1.00 49.76	C
ATOM	785	CD	ARG	752	5.938	20.434	2.649	1.00 48.23	C
ATOM	786	NE	ARG	752	5.382	21.773	2.483	1.00 45.23	N
ATOM	788	CZ	ARG	752	5.013	22.572	3.490	1.00 52.17	C
ATOM	789	NH1	ARG	752	5.131	22.175	4.764	1.00 33.80	N
ATOM	792	NH2	ARG	752	4.536	23.785	3.223	1.00 49.84	N
ATOM	795	C	ARG	752	10.257	21.740	0.602	1.00 44.18	C
ATOM	796	O	ARG	752	10.522	21.048	-0.380	1.00 43.20	O
ATOM	797	N	SER	753	10.441	23.058	0.624	1.00 38.26	N
ATOM	799	CA	SER	753	10.998	23.733	-0.523	1.00 35.26	C
ATOM	800	CB	SER	753	10.798	25.233	-0.444	1.00 33.49	C
ATOM	801	OG	SER	753	9.414	25.514	-0.453	1.00 36.06	O
ATOM	803	C	SER	753	12.453	23.400	-0.707	1.00 35.66	C
ATOM	804	O	SER	753	12.973	23.538	-1.807	1.00 43.18	O
ATOM	805	N	PHE	754	13.113	22.938	0.343	1.00 33.77	N
ATOM	807	CA	PHE	754	14.523	22.575	0.224	1.00 41.59	C
ATOM	808	CB	PHE	754	15.242	22.702	1.564	1.00 39.18	C
ATOM	809	CG	PHE	754	16.668	22.204	1.540	1.00 40.02	C

FIG. 6 CONT'D

ATOM	810	CD1	PHE	754	17.596	22.746	0.645	1.00	48.31	C
ATOM	811	CD2	PHE	754	17.086	21.202	2.423	1.00	36.75	C
ATOM	812	CE1	PHE	754	18.923	22.311	0.635	1.00	47.66	C
ATOM	813	CE2	PHE	754	18.411	20.757	2.432	1.00	41.02	C
ATOM	814	CZ	PHE	754	19.333	21.313	1.532	1.00	50.13	C
ATOM	815	C	PHE	754	14.709	21.153	-0.316	1.00	49.14	C
ATOM	816	O	PHE	754	15.524	20.919	-1.211	1.00	48.97	O
ATOM	817	N	THR	755	13.948	20.208	0.225	1.00	53.24	N
ATOM	819	CA	THR	755	14.053	18.818	-0.197	1.00	53.33	C
ATOM	820	CB	THR	755	13.596	17.830	0.934	1.00	45.98	C
ATOM	821	OG1	THR	755	12.221	18.055	1.245	1.00	49.35	O
ATOM	823	CG2	THR	755	14.405	18.033	2.190	1.00	40.03	C
ATOM	824	C	THR	755	13.287	18.474	-1.478	1.00	54.87	C
ATOM	825	O	THR	755	13.554	17.431	-2.068	1.00	57.41	O
ATOM	826	N	ASN	756	12.360	19.336	-1.911	1.00	52.97	N
ATOM	828	CA	ASN	756	11.539	19.044	-3.097	1.00	56.15	C
ATOM	829	CB	ASN	756	10.019	19.124	-2.769	1.00	60.43	C
ATOM	830	CG	ASN	756	9.504	17.959	-1.869	1.00	57.82	C
ATOM	831	OD1	ASN	756	10.123	16.909	-1.763	1.00	55.71	O
ATOM	832	ND2	ASN	756	8.354	18.169	-1.234	1.00	56.46	N
ATOM	835	C	ASN	756	11.821	19.826	-4.394	1.00	55.33	C
ATOM	836	O	ASN	756	11.705	19.257	-5.481	1.00	54.81	O
ATOM	837	N	VAL	757	12.155	21.115	-4.293	1.00	54.53	N
ATOM	839	CA	VAL	757	12.427	21.962	-5.470	1.00	50.64	C
ATOM	840	CB	VAL	757	11.239	22.943	-5.756	1.00	50.94	C
ATOM	841	CG1	VAL	757	9.927	22.177	-5.892	1.00	53.22	C
ATOM	842	CG2	VAL	757	11.125	23.998	-4.660	1.00	54.28	C
ATOM	843	C	VAL	757	13.732	22.776	-5.370	1.00	47.30	C
ATOM	844	O	VAL	757	13.903	23.786	-6.053	1.00	48.03	O
ATOM	845	N	ASN	758	14.676	22.274	-4.582	1.00	53.28	N
ATOM	847	CA	ASN	758	15.977	22.917	-4.340	1.00	61.04	C
ATOM	848	CB	ASN	758	17.026	22.499	-5.388	1.00	63.98	C
ATOM	849	CG	ASN	758	18.440	22.442	-4.813	1.00	62.08	C
ATOM	850	OD1	ASN	758	18.681	22.852	-3.679	0.00	62.62	O
ATOM	851	ND2	ASN	758	19.369	21.908	-5.590	0.00	62.48	N
ATOM	854	C	ASN	758	15.937	24.448	-4.140	1.00	63.53	C
ATOM	855	O	ASN	758	16.674	25.191	-4.802	1.00	65.98	O
ATOM	856	N	SER	759	14.999	24.879	-3.281	1.00	63.72	N
ATOM	858	CA	SER	759	14.763	26.267	-2.849	1.00	61.29	C
ATOM	859	CB	SER	759	15.939	26.770	-1.995	1.00	60.64	C
ATOM	860	OG	SER	759	16.080	26.018	-0.799	1.00	55.92	O
ATOM	862	C	SER	759	14.379	27.351	-3.849	1.00	66.13	C
ATOM	863	O	SER	759	14.067	28.472	-3.443	1.00	71.37	O
ATOM	864	N	ARG	760	14.388	27.045	-5.140	1.00	64.35	N
ATOM	866	CA	ARG	760	14.041	28.064	-6.109	1.00	59.78	C
ATOM	867	CB	ARG	760	14.492	27.658	-7.507	1.00	69.19	C
ATOM	868	CG	ARG	760	14.046	26.283	-7.883	1.00	73.58	C
ATOM	869	CD	ARG	760	13.925	26.094	-9.381	1.00	78.27	C
ATOM	870	NE	ARG	760	13.214	24.847	-9.635	1.00	80.85	N
ATOM	872	CZ	ARG	760	13.642	23.646	-9.246	1.00	80.46	C
ATOM	873	NH1	ARG	760	14.801	23.528	-8.597	1.00	79.19	N
ATOM	876	NH2	ARG	760	12.853	22.584	-9.388	1.00	76.84	N
ATOM	879	C	ARG	760	12.551	28.416	-6.070	1.00	55.67	C
ATOM	880	O	ARG	760	12.186	29.563	-6.345	1.00	60.84	O
ATOM	881	N	MET	761	11.701	27.453	-5.707	1.00	46.97	N
ATOM	883	CA	MET	761	10.256	27.695	-5.622	1.00	41.01	C

FIG. 6 CONT'D

ATOM	884	CB	MET	761	9.496	26.827	-6.612	1.00	38.49	C
ATOM	885	CG	MET	761	9.926	27.040	-8.034	1.00	42.52	C
ATOM	886	SD	MET	761	8.981	25.994	-9.104	1.00	50.12	S
ATOM	887	CE	MET	761	10.000	24.558	-9.111	1.00	43.61	C
ATOM	888	C	MET	761	9.744	27.418	-4.222	1.00	37.53	C
ATOM	889	O	MET	761	10.451	26.824	-3.412	1.00	38.47	O
ATOM	890	N	LEU	762	8.526	27.860	-3.930	1.00	35.00	N
ATOM	892	CA	LEU	762	7.949	27.638	-2.614	1.00	36.81	C
ATOM	893	CB	LEU	762	7.344	28.912	-2.048	1.00	39.16	C
ATOM	894	CG	LEU	762	8.366	30.021	-1.827	1.00	43.49	C
ATOM	895	CD1	LEU	762	7.670	31.178	-1.169	1.00	45.89	C
ATOM	896	CD2	LEU	762	9.498	29.530	-0.952	1.00	44.69	C
ATOM	897	C	LEU	762	6.902	26.548	-2.664	1.00	41.13	C
ATOM	898	O	LEU	762	5.821	26.739	-3.243	1.00	36.62	O
ATOM	899	N	TYR	763	7.245	25.419	-2.033	1.00	44.41	N
ATOM	901	CA	TYR	763	6.422	24.209	-1.963	1.00	39.75	C
ATOM	902	CB	TYR	763	7.323	22.968	-1.831	1.00	47.60	C
ATOM	903	CG	TYR	763	6.713	21.644	-2.309	1.00	61.61	C
ATOM	904	CD1	TYR	763	5.701	21.002	-1.579	1.00	67.78	C
ATOM	905	CE1	TYR	763	5.164	19.770	-1.998	1.00	63.34	C
ATOM	906	CD2	TYR	763	7.174	21.015	-3.476	1.00	62.67	C
ATOM	907	CE2	TYR	763	6.639	19.778	-3.897	1.00	59.80	C
ATOM	908	CZ	TYR	763	5.634	19.173	-3.149	1.00	62.05	C
ATOM	909	OH	TYR	763	5.066	17.995	-3.558	1.00	63.40	O
ATOM	911	C	TYR	763	5.412	24.241	-0.839	1.00	36.53	C
ATOM	912	O	TYR	763	5.504	23.487	0.129	1.00	36.31	O
ATOM	913	N	PHE	764	4.445	25.130	-0.958	1.00	37.20	N
ATOM	915	CA	PHE	764	3.409	25.221	0.042	1.00	38.87	C
ATOM	916	CB	PHE	764	2.441	26.350	-0.321	1.00	34.03	C
ATOM	917	CG	PHE	764	3.048	27.695	-0.225	1.00	29.36	C
ATOM	918	CD1	PHE	764	3.129	28.510	-1.328	1.00	37.55	C
ATOM	919	CD2	PHE	764	3.571	28.142	0.976	1.00	32.46	C
ATOM	920	CE1	PHE	764	3.727	29.759	-1.236	1.00	39.68	C
ATOM	921	CE2	PHE	764	4.169	29.384	1.076	1.00	35.80	C
ATOM	922	CZ	PHE	764	4.247	30.196	-0.033	1.00	29.54	C
ATOM	923	C	PHE	764	2.681	23.864	0.164	1.00	47.03	C
ATOM	924	O	PHE	764	2.506	23.333	1.263	1.00	48.96	O
ATOM	925	N	ALA	765	2.314	23.286	-0.978	1.00	56.26	N
ATOM	927	CA	ALA	765	1.608	21.999	-1.049	1.00	51.43	C
ATOM	928	CB	ALA	765	0.105	22.232	-0.959	1.00	47.80	C
ATOM	929	C	ALA	765	1.969	21.343	-2.386	1.00	51.42	C
ATOM	930	O	ALA	765	2.449	22.022	-3.289	1.00	51.71	O
ATOM	931	N	PRO	766	1.766	20.021	-2.533	1.00	52.86	N
ATOM	932	CD	PRO	766	1.237	19.002	-1.617	1.00	57.23	C
ATOM	933	CA	PRO	766	2.120	19.407	-3.813	1.00	50.96	C
ATOM	934	CB	PRO	766	1.721	17.949	-3.604	1.00	57.00	C
ATOM	935	CG	PRO	766	1.899	17.761	-2.133	1.00	58.08	C
ATOM	936	C	PRO	766	1.359	20.040	-4.970	1.00	48.25	C
ATOM	937	O	PRO	766	1.893	20.144	-6.082	1.00	44.31	O
ATOM	938	N	ASP	767	0.128	20.479	-4.707	1.00	41.59	N
ATOM	940	CA	ASP	767	-0.681	21.119	-5.743	1.00	47.13	C
ATOM	941	CB	ASP	767	-2.073	20.485	-5.785	1.00	48.65	C
ATOM	942	CG	ASP	767	-2.833	20.667	-4.505	1.00	51.77	C
ATOM	943	OD1	ASP	767	-4.071	20.839	-4.573	1.00	59.43	O
ATOM	944	OD2	ASP	767	-2.205	20.619	-3.431	1.00	54.76	O
ATOM	945	C	ASP	767	-0.774	22.666	-5.645	1.00	51.59	C

FIG. 6 CONT'D

ATOM	946	O	ASP	767	-1.618	23.311	-6.292	1.00 55.70	O
ATOM	947	N	LEU	768	0.148	23.255	-4.893	1.00 48.07	N
ATOM	949	CA	LEU	768	0.196	24.697	-4.719	1.00 47.04	C
ATOM	950	CB	LEU	768	-0.574	25.108	-3.450	1.00 51.86	C
ATOM	951	CG	LEU	768	-0.631	26.580	-3.002	1.00 50.53	C
ATOM	952	CD1	LEU	768	-1.328	27.390	-4.062	1.00 47.97	C
ATOM	953	CD2	LEU	768	-1.376	26.701	-1.702	1.00 46.42	C
ATOM	954	C	LEU	768	1.658	25.080	-4.564	1.00 49.99	C
ATOM	955	O	LEU	768	2.141	25.212	-3.436	1.00 53.64	O
ATOM	956	N	VAL	769	2.387	25.176	-5.676	1.00 48.70	N
ATOM	958	CA	VAL	769	3.796	25.575	-5.620	1.00 48.86	C
ATOM	959	CB	VAL	769	4.728	24.572	-6.321	1.00 50.85	C
ATOM	960	CG1	VAL	769	6.181	25.049	-6.216	1.00 53.54	C
ATOM	961	CG2	VAL	769	4.581	23.208	-5.687	1.00 53.42	C
ATOM	962	C	VAL	769	3.954	26.933	-6.287	1.00 47.94	C
ATOM	963	O	VAL	769	3.352	27.190	-7.335	1.00 49.55	O
ATOM	964	N	PHE	770	4.734	27.808	-5.668	1.00 43.61	N
ATOM	966	CA	PHE	770	4.935	29.124	-6.230	1.00 40.71	C
ATOM	967	CB	PHE	770	4.939	30.197	-5.147	1.00 41.24	C
ATOM	968	CG	PHE	770	3.582	30.650	-4.753	1.00 39.60	C
ATOM	969	CD1	PHE	770	2.489	29.803	-4.896	1.00 40.94	C
ATOM	970	CD2	PHE	770	3.391	31.916	-4.220	1.00 35.47	C
ATOM	971	CE1	PHE	770	1.216	30.208	-4.515	1.00 39.80	C
ATOM	972	CE2	PHE	770	2.123	32.332	-3.834	1.00 37.83	C
ATOM	973	CZ	PHE	770	1.027	31.476	-3.980	1.00 36.48	C
ATOM	974	C	PHE	770	6.179	29.276	-7.044	1.00 39.27	C
ATOM	975	O	PHE	770	7.291	29.151	-6.531	1.00 38.13	O
ATOM	976	N	ASN	771	5.988	29.397	-8.345	1.00 38.22	N
ATOM	978	CA	ASN	771	7.113	29.673	-9.219	1.00 39.10	C
ATOM	979	CB	ASN	771	6.834	29.268	-10.685	1.00 33.28	C
ATOM	980	CG	ASN	771	5.384	29.492	-11.110	1.00 35.37	C
ATOM	981	OD1	ASN	771	4.656	30.309	-10.546	1.00 45.29	O
ATOM	982	ND2	ASN	771	4.956	28.737	-12.094	1.00 41.79	N
ATOM	985	C	ASN	771	7.181	31.196	-9.066	1.00 43.17	C
ATOM	986	O	ASN	771	6.341	31.785	-8.345	1.00 39.83	O
ATOM	987	N	GLU	772	8.166	31.836	-9.694	1.00 43.13	N
ATOM	989	CA	GLU	772	8.264	33.285	-9.605	1.00 42.44	C
ATOM	990	CB	GLU	772	9.541	33.815	-10.274	1.00 52.58	C
ATOM	991	CG	GLU	772	10.814	33.657	-9.401	1.00 58.43	C
ATOM	992	CD	GLU	772	11.791	34.850	-9.483	1.00 56.79	C
ATOM	993	OE1	GLU	772	12.654	34.974	-8.583	1.00 61.19	O
ATOM	994	OE2	GLU	772	11.719	35.655	-10.434	1.00 55.14	O
ATOM	995	C	GLU	772	7.015	33.997	-10.136	1.00 45.81	C
ATOM	996	O	GLU	772	6.615	35.016	-9.579	1.00 53.45	O
ATOM	997	N	TYR	773	6.354	33.454	-11.157	1.00 39.45	N
ATOM	999	CA	TYR	773	5.147	34.117	-11.659	1.00 38.06	C
ATOM	1000	CB	TYR	773	4.563	33.425	-12.907	1.00 37.63	C
ATOM	1001	CG	TYR	773	3.266	34.033	-13.417	1.00 38.44	C
ATOM	1002	CD1	TYR	773	3.248	35.277	-14.059	1.00 36.94	C
ATOM	1003	CE1	TYR	773	2.038	35.883	-14.459	1.00 34.34	C
ATOM	1004	CD2	TYR	773	2.043	33.397	-13.197	1.00 40.91	C
ATOM	1005	CE2	TYR	773	0.833	33.990	-13.595	1.00 46.98	C
ATOM	1006	CZ	TYR	773	0.835	35.235	-14.223	1.00 42.85	C
ATOM	1007	OH	TYR	773	-0.361	35.824	-14.599	1.00 42.16	O
ATOM	1009	C	TYR	773	4.088	34.215	-10.565	1.00 38.71	C
ATOM	1010	O	TYR	773	3.493	35.271	-10.391	1.00 41.42	O

FIG. 6 CONT'D

ATOM	1011	N	ARG	774	3.864	33.137	-9.817	1.00	43.58	N
ATOM	1013	CA	ARG	774	2.863	33.146	-8.751	1.00	41.94	C
ATOM	1014	CB	ARG	774	2.580	31.748	-8.252	1.00	46.64	C
ATOM	1015	CG	ARG	774	1.421	31.121	-8.923	1.00	45.32	C
ATOM	1016	CD	ARG	774	1.735	29.667	-9.102	1.00	47.16	C
ATOM	1017	NE	ARG	774	0.588	28.968	-9.642	1.00	43.73	N
ATOM	1019	CZ	ARG	774	0.344	27.682	-9.445	1.00	41.94	C
ATOM	1020	NH1	ARG	774	1.183	26.954	-8.717	1.00	42.65	N
ATOM	1023	NH2	ARG	774	-0.753	27.136	-9.952	1.00	39.92	N
ATOM	1026	C	ARG	774	3.216	34.035	-7.578	1.00	41.03	C
ATOM	1027	O	ARG	774	2.330	34.701	-7.032	1.00	43.75	O
ATOM	1028	N	MET	775	4.486	34.023	-7.168	1.00	34.68	N
ATOM	1030	CA	MET	775	4.955	34.877	-6.069	1.00	38.36	C
ATOM	1031	CB	MET	775	6.485	34.839	-5.975	1.00	33.18	C
ATOM	1032	CG	MET	775	7.046	33.622	-5.276	1.00	24.32	C
ATOM	1033	SD	MET	775	8.813	33.416	-5.539	1.00	40.19	S
ATOM	1034	CE	MET	775	9.443	34.965	-4.970	1.00	48.34	C
ATOM	1035	C	MET	775	4.496	36.328	-6.332	1.00	41.88	C
ATOM	1036	O	MET	775	4.119	37.065	-5.416	1.00	41.28	O
ATOM	1037	N	HIS	776	4.484	36.695	-7.608	1.00	46.87	N
ATOM	1039	CA	HIS	776	4.065	38.006	-8.065	1.00	41.06	C
ATOM	1040	CB	HIS	776	4.804	38.351	-9.348	1.00	45.79	C
ATOM	1041	CG	HIS	776	4.486	39.712	-9.873	1.00	44.99	C
ATOM	1042	CD2	HIS	776	5.167	40.879	-9.788	1.00	44.43	C
ATOM	1043	ND1	HIS	776	3.327	39.992	-10.560	1.00	46.34	N
ATOM	1045	CE1	HIS	776	3.300	41.270	-10.877	1.00	44.55	C
ATOM	1046	NE2	HIS	776	4.406	41.833	-10.419	1.00	49.86	N
ATOM	1048	C	HIS	776	2.568	38.136	-8.311	1.00	43.18	C
ATOM	1049	O	HIS	776	1.969	39.153	-7.991	1.00	48.98	O
ATOM	1050	N	LYS	777	1.964	37.143	-8.938	1.00	46.29	N
ATOM	1052	CA	LYS	777	0.542	37.214	-9.220	1.00	48.46	C
ATOM	1053	CB	LYS	777	0.128	36.042	-10.126	1.00	50.10	C
ATOM	1054	CG	LYS	777	-1.193	36.233	-10.872	1.00	58.08	C
ATOM	1055	CD	LYS	777	-1.161	37.460	-11.791	1.00	65.16	C
ATOM	1056	CE	LYS	777	-2.090	38.590	-11.301	1.00	75.26	C
ATOM	1057	NZ	LYS	777	-3.524	38.363	-11.635	1.00	77.33	N
ATOM	1061	C	LYS	777	-0.276	37.241	-7.920	1.00	49.12	C
ATOM	1062	O	LYS	777	-1.356	37.835	-7.869	1.00	53.96	O
ATOM	1063	N	SER	778	0.249	36.616	-6.870	1.00	50.25	N
ATOM	1065	CA	SER	778	-0.432	36.551	-5.571	1.00	48.63	C
ATOM	1066	CB	SER	778	0.116	35.397	-4.761	1.00	42.58	C
ATOM	1067	OG	SER	778	1.446	35.715	-4.386	1.00	43.83	O
ATOM	1069	C	SER	778	-0.193	37.808	-4.756	1.00	53.35	C
ATOM	1070	O	SER	778	-0.827	38.019	-3.727	1.00	57.00	O
ATOM	1071	N	ARG	779	0.842	38.546	-5.141	1.00	58.37	N
ATOM	1073	CA	ARG	779	1.242	39.798	-4.491	1.00	56.74	C
ATOM	1074	CB	ARG	779	0.081	40.799	-4.461	1.00	57.70	C
ATOM	1075	CG	ARG	779	-0.472	41.124	-5.841	1.00	56.33	C
ATOM	1076	CD	ARG	779	-1.603	42.120	-5.735	1.00	58.79	C
ATOM	1077	NE	ARG	779	-2.471	42.088	-6.907	1.00	62.79	N
ATOM	1079	CZ	ARG	779	-3.095	43.150	-7.397	1.00	61.40	C
ATOM	1080	NH1	ARG	779	-2.935	44.337	-6.824	1.00	62.02	N
ATOM	1083	NH2	ARG	779	-3.912	43.007	-8.426	1.00	65.13	N
ATOM	1086	C	ARG	779	1.901	39.668	-3.113	1.00	54.76	C
ATOM	1087	O	ARG	779	1.801	40.580	-2.276	1.00	51.96	O
ATOM	1088	N	MET	780	2.600	38.551	-2.897	1.00	46.79	N

FIG. 6 CONT'D

ATOM	1090	CA	MET	780	3.323	38.334	-1.650	1.00	42.92	C
ATOM	1091	CB	MET	780	2.953	37.015	-1.005	1.00	45.45	C
ATOM	1092	CG	MET	780	1.530	36.831	-0.596	1.00	54.10	C
ATOM	1093	SD	MET	780	1.554	35.622	0.748	1.00	62.75	S
ATOM	1094	CE	MET	780	2.616	34.289	0.007	1.00	62.66	C
ATOM	1095	C	MET	780	4.773	38.214	-2.049	1.00	41.04	C
ATOM	1096	O	MET	780	5.595	37.686	-1.311	1.00	43.38	O
ATOM	1097	N	TYR	781	5.092	38.712	-3.229	1.00	39.62	N
ATOM	1099	CA	TYR	781	6.429	38.610	-3.744	1.00	33.06	C
ATOM	1100	CB	TYR	781	6.581	39.428	-5.019	1.00	33.87	C
ATOM	1101	CG	TYR	781	7.782	38.995	-5.819	1.00	46.69	C
ATOM	1102	CD1	TYR	781	7.651	38.203	-6.952	1.00	48.14	C
ATOM	1103	CE1	TYR	781	8.778	37.756	-7.644	1.00	46.86	C
ATOM	1104	CD2	TYR	781	9.063	39.330	-5.400	1.00	53.38	C
ATOM	1105	CE2	TYR	781	10.184	38.887	-6.071	1.00	50.46	C
ATOM	1106	CZ	TYR	781	10.051	38.105	-7.190	1.00	51.34	C
ATOM	1107	OH	TYR	781	11.207	37.679	-7.825	1.00	55.86	O
ATOM	1109	C	TYR	781	7.532	38.923	-2.753	1.00	33.20	C
ATOM	1110	O	TYR	781	8.499	38.166	-2.682	1.00	40.06	O
ATOM	1111	N	SER	782	7.419	40.009	-1.986	1.00	39.72	N
ATOM	1113	CA	SER	782	8.492	40.346	-1.009	1.00	46.33	C
ATOM	1114	CB	SER	782	8.364	41.780	-0.472	1.00	44.39	C
ATOM	1115	OG	SER	782	7.042	42.049	-0.044	1.00	52.83	O
ATOM	1117	C	SER	782	8.597	39.361	0.159	1.00	38.58	C
ATOM	1118	O	SER	782	9.697	39.007	0.604	1.00	34.19	O
ATOM	1119	N	GLN	783	7.453	38.904	0.650	1.00	36.42	N
ATOM	1121	CA	GLN	783	7.486	37.948	1.736	1.00	43.09	C
ATOM	1122	CB	GLN	783	6.102	37.717	2.321	1.00	42.73	C
ATOM	1123	CG	GLN	783	5.538	38.915	3.059	1.00	48.39	C
ATOM	1124	CD	GLN	783	5.113	40.045	2.137	1.00	50.96	C
ATOM	1125	OE1	GLN	783	4.504	39.831	1.083	1.00	53.94	O
ATOM	1126	NE2	GLN	783	5.430	41.260	2.538	1.00	52.89	N
ATOM	1129	C	GLN	783	8.040	36.661	1.160	1.00	41.26	C
ATOM	1130	O	GLN	783	8.980	36.075	1.709	1.00	47.55	O
ATOM	1131	N	CYS	784	7.532	36.300	-0.015	1.00	36.76	N
ATOM	1133	CA	CYS	784	7.945	35.084	-0.710	1.00	35.38	C
ATOM	1134	CB	CYS	784	7.244	34.989	-2.066	1.00	31.26	C
ATOM	1135	SG	CYS	784	5.513	34.425	-1.949	1.00	42.23	S
ATOM	1136	C	CYS	784	9.456	35.006	-0.859	1.00	33.10	C
ATOM	1137	O	CYS	784	10.073	33.978	-0.568	1.00	39.32	O
ATOM	1138	N	VAL	785	10.060	36.132	-1.199	1.00	33.87	N
ATOM	1140	CA	VAL	785	11.491	36.173	-1.363	1.00	31.80	C
ATOM	1141	CB	VAL	785	11.928	37.502	-1.962	1.00	37.92	C
ATOM	1142	CG1	VAL	785	13.417	37.484	-2.236	1.00	35.87	C
ATOM	1143	CG2	VAL	785	11.171	37.748	-3.264	1.00	33.21	C
ATOM	1144	C	VAL	785	12.149	35.937	-0.019	1.00	33.12	C
ATOM	1145	O	VAL	785	13.164	35.267	0.051	1.00	35.91	O
ATOM	1146	N	ARG	786	11.556	36.461	1.052	1.00	36.61	N
ATOM	1148	CA	ARG	786	12.091	36.278	2.406	1.00	38.66	C
ATOM	1149	CB	ARG	786	11.343	37.175	3.407	1.00	44.04	C
ATOM	1150	CG	ARG	786	11.732	38.650	3.320	1.00	47.85	C
ATOM	1151	CD	ARG	786	12.880	38.968	4.255	1.00	50.22	C
ATOM	1152	NE	ARG	786	12.397	39.082	5.635	1.00	62.62	N
ATOM	1154	CZ	ARG	786	13.172	39.167	6.719	1.00	58.03	C
ATOM	1155	NH1	ARG	786	14.494	39.134	6.609	1.00	61.23	N
ATOM	1158	NH2	ARG	786	12.621	39.385	7.908	1.00	54.77	N

FIG. 6 CONT'D

ATOM	1161	C	ARG	786	12.037	34.801	2.831	1.00 36.30	C
ATOM	1162	O	ARG	786	13.008	34.249	3.362	1.00 38.29	O
ATOM	1163	N	MET	787	10.919	34.150	2.553	1.00 32.73	N
ATOM	1165	CA	MET	787	10.763	32.746	2.883	1.00 34.16	C
ATOM	1166	CB	MET	787	9.331	32.315	2.621	1.00 27.15	C
ATOM	1167	CG	MET	787	8.337	33.046	3.449	1.00 32.77	C
ATOM	1168	SD	MET	787	6.714	32.334	3.317	1.00 46.02	S
ATOM	1169	CE	MET	787	6.063	33.236	2.001	1.00 31.94	C
ATOM	1170	C	MET	787	11.733	31.878	2.066	1.00 38.91	C
ATOM	1171	O	MET	787	12.229	30.846	2.539	1.00 43.10	O
ATOM	1172	N	ARG	788	11.999	32.296	0.835	1.00 39.06	N
ATOM	1174	CA	ARG	788	12.902	31.570	-0.035	1.00 34.24	C
ATOM	1175	CB	ARG	788	12.790	32.122	-1.446	1.00 39.81	C
ATOM	1176	CG	ARG	788	13.263	31.196	-2.528	1.00 45.01	C
ATOM	1177	CD	ARG	788	12.846	31.727	-3.887	1.00 54.21	C
ATOM	1178	NE	ARG	788	13.605	32.913	-4.290	1.00 63.42	N
ATOM	1180	CZ	ARG	788	13.340	33.620	-5.386	1.00 68.54	C
ATOM	1181	NH1	ARG	788	12.329	33.261	-6.163	1.00 72.57	N
ATOM	1184	NH2	ARG	788	14.126	34.630	-5.752	1.00 72.25	N
ATOM	1187	C	ARG	788	14.323	31.664	0.502	1.00 34.59	C
ATOM	1188	O	ARG	788	15.119	30.742	0.332	1.00 37.27	O
ATOM	1189	N	HIS	789	14.636	32.759	1.191	1.00 40.92	N
ATOM	1191	CA	HIS	789	15.973	32.916	1.784	1.00 53.01	C
ATOM	1192	CB	HIS	789	16.114	34.232	2.575	1.00 64.44	C
ATOM	1193	CG	HIS	789	16.334	35.456	1.739	1.00 74.91	C
ATOM	1194	CD2	HIS	789	16.051	36.759	1.982	1.00 74.30	C
ATOM	1195	ND1	HIS	789	16.916	35.419	0.490	1.00 80.32	N
ATOM	1197	CE1	HIS	789	16.982	36.648	-0.001	1.00 78.33	C
ATOM	1198	NE2	HIS	789	16.465	37.481	0.886	1.00 74.90	N
ATOM	1200	C	HIS	789	16.107	31.777	2.782	1.00 54.43	C
ATOM	1201	O	HIS	789	17.066	31.000	2.730	1.00 50.35	O
ATOM	1202	N	LEU	790	15.112	31.700	3.674	1.00 56.83	N
ATOM	1204	CA	LEU	790	15.018	30.684	4.731	1.00 50.54	C
ATOM	1205	CB	LEU	790	13.660	30.757	5.427	1.00 47.65	C
ATOM	1206	CG	LEU	790	13.455	29.853	6.634	1.00 49.09	C
ATOM	1207	CD1	LEU	790	14.230	30.415	7.825	1.00 56.25	C
ATOM	1208	CD2	LEU	790	11.970	29.760	6.962	1.00 46.26	C
ATOM	1209	C	LEU	790	15.194	29.297	4.140	1.00 45.95	C
ATOM	1210	O	LEU	790	16.076	28.551	4.573	1.00 43.16	O
ATOM	1211	N	SER	791	14.388	28.963	3.130	1.00 38.77	N
ATOM	1213	CA	SER	791	14.516	27.661	2.501	1.00 35.86	C
ATOM	1214	CB	SER	791	13.515	27.479	1.363	1.00 39.07	C
ATOM	1215	OG	SER	791	13.974	28.090	0.177	1.00 55.38	O
ATOM	1217	C	SER	791	15.951	27.507	2.010	1.00 37.61	C
ATOM	1218	O	SER	791	16.533	26.432	2.127	1.00 42.51	O
ATOM	1219	N	GLN	792	16.563	28.585	1.541	1.00 38.43	N
ATOM	1221	CA	GLN	792	17.938	28.481	1.086	1.00 43.65	C
ATOM	1222	CB	GLN	792	18.297	29.652	0.201	1.00 43.96	C
ATOM	1223	CG	GLN	792	17.455	29.723	-1.021	1.00 50.40	C
ATOM	1224	CD	GLN	792	17.516	31.082	-1.648	1.00 56.80	C
ATOM	1225	OE1	GLN	792	17.275	32.081	-0.975	1.00 59.46	O
ATOM	1226	NE2	GLN	792	17.852	31.142	-2.938	1.00 56.24	N
ATOM	1229	C	GLN	792	18.978	28.304	2.201	1.00 46.43	C
ATOM	1230	O	GLN	792	20.049	27.761	1.951	1.00 53.03	O
ATOM	1231	N	GLU	793	18.684	28.734	3.424	1.00 46.80	N
ATOM	1233	CA	GLU	793	19.658	28.561	4.510	1.00 46.06	C

FIG. 6 CONT'D

ATOM	1234	CB	GLU	793	19.214	29.248	5.814	1.00	51.06	C
ATOM	1235	CG	GLU	793	18.949	30.772	5.734	1.00	67.15	C
ATOM	1236	CD	GLU	793	20.212	31.644	5.762	1.00	74.35	C
ATOM	1237	OE1	GLU	793	21.328	31.098	5.703	1.00	72.15	O
ATOM	1238	OE2	GLU	793	20.083	32.894	5.837	1.00	83.11	O
ATOM	1239	C	GLU	793	19.852	27.078	4.787	1.00	40.74	C
ATOM	1240	O	GLU	793	20.972	26.632	5.000	1.00	41.28	O
ATOM	1241	N	PHE	794	18.771	26.302	4.760	1.00	38.60	N
ATOM	1243	CA	PHE	794	18.862	24.866	5.031	1.00	36.65	C
ATOM	1244	CB	PHE	794	17.562	24.160	4.686	1.00	32.29	C
ATOM	1245	CG	PHE	794	16.462	24.410	5.669	1.00	37.63	C
ATOM	1246	CD1	PHE	794	16.704	24.358	7.030	1.00	37.22	C
ATOM	1247	CD2	PHE	794	15.173	24.718	5.229	1.00	43.04	C
ATOM	1248	CE1	PHE	794	15.665	24.605	7.945	1.00	35.06	C
ATOM	1249	CE2	PHE	794	14.126	24.969	6.140	1.00	37.46	C
ATOM	1250	CZ	PHE	794	14.376	24.913	7.494	1.00	27.46	C
ATOM	1251	C	PHE	794	19.960	24.277	4.206	1.00	40.69	C
ATOM	1252	O	PHE	794	20.761	23.478	4.690	1.00	41.76	O
ATOM	1253	N	GLY	795	20.018	24.729	2.963	1.00	51.69	N
ATOM	1255	CA	GLY	795	21.033	24.260	2.040	1.00	57.61	C
ATOM	1256	C	GLY	795	22.440	24.695	2.391	1.00	58.51	C
ATOM	1257	O	GLY	795	23.338	23.850	2.481	1.00	54.63	O
ATOM	1258	N	TRP	796	22.625	25.994	2.624	1.00	56.85	N
ATOM	1260	CA	TRP	796	23.942	26.504	2.944	1.00	61.47	C
ATOM	1261	CB	TRP	796	23.966	28.039	2.770	1.00	77.04	C
ATOM	1262	CG	TRP	796	24.441	28.924	3.938	1.00	99.05	C
ATOM	1263	CD2	TRP	796	25.693	28.847	4.686	1.00	107.94	C
ATOM	1264	CE2	TRP	796	25.701	29.929	5.606	1.00	109.90	C
ATOM	1265	CE3	TRP	796	26.801	27.976	4.667	1.00	108.72	C
ATOM	1266	CD1	TRP	796	23.779	30.018	4.436	1.00	103.16	C
ATOM	1267	NE1	TRP	796	24.528	30.622	5.430	1.00	107.43	N
ATOM	1269	CZ2	TRP	796	26.778	30.157	6.503	1.00	110.69	C
ATOM	1270	CZ3	TRP	796	27.871	28.204	5.561	1.00	110.67	C
ATOM	1271	CH2	TRP	796	27.845	29.286	6.462	1.00	111.09	C
ATOM	1272	C	TRP	796	24.433	25.986	4.301	1.00	59.21	C
ATOM	1273	O	TRP	796	25.614	25.649	4.469	1.00	55.17	O
ATOM	1274	N	LEU	797	23.500	25.779	5.221	1.00	56.75	N
ATOM	1276	CA	LEU	797	23.851	25.286	6.546	1.00	54.04	C
ATOM	1277	CB	LEU	797	22.839	25.782	7.583	1.00	52.49	C
ATOM	1278	CG	LEU	797	23.080	27.184	8.151	1.00	42.33	C
ATOM	1279	CD1	LEU	797	21.835	27.737	8.827	1.00	39.02	C
ATOM	1280	CD2	LEU	797	24.229	27.123	9.128	1.00	43.89	C
ATOM	1281	C	LEU	797	24.012	23.767	6.640	1.00	56.56	C
ATOM	1282	O	LEU	797	24.629	23.277	7.587	1.00	62.03	O
ATOM	1283	N	GLN	798	23.462	23.020	5.684	1.00	53.42	N
ATOM	1285	CA	GLN	798	23.560	21.561	5.708	1.00	57.87	C
ATOM	1286	CB	GLN	798	25.028	21.103	5.774	1.00	67.87	C
ATOM	1287	CG	GLN	798	25.773	21.088	4.438	1.00	83.30	C
ATOM	1288	CD	GLN	798	27.115	20.345	4.507	1.00	91.19	C
ATOM	1289	OE1	GLN	798	27.910	20.564	5.428	1.00	96.98	O
ATOM	1290	NE2	GLN	798	27.368	19.463	3.532	1.00	87.09	N
ATOM	1293	C	GLN	798	22.788	20.960	6.890	1.00	54.98	C
ATOM	1294	O	GLN	798	23.268	20.039	7.571	1.00	53.85	O
ATOM	1295	N	ILE	799	21.597	21.494	7.131	1.00	49.17	N
ATOM	1297	CA	ILE	799	20.728	21.040	8.219	1.00	45.76	C
ATOM	1298	CB	ILE	799	19.414	21.894	8.258	1.00	38.57	C

FIG. 6 CONT'D

ATOM	1299	CG2	ILE	799	18.532	21.450	9.379	1.00	36.81	C
ATOM	1300	CG1	ILE	799	19.733	23.388	8.383	1.00	36.16	C
ATOM	1301	CD1	ILE	799	20.686	23.691	9.480	1.00	27.19	C
ATOM	1302	C	ILE	799	20.348	19.545	8.071	1.00	47.10	C
ATOM	1303	O	ILE	799	19.766	19.135	7.059	1.00	40.12	O
ATOM	1304	N	THR	800	20.735	18.725	9.045	1.00	46.19	N
ATOM	1306	CA	THR	800	20.386	17.310	9.026	1.00	47.55	C
ATOM	1307	CB	THR	800	21.222	16.474	10.060	1.00	47.29	C
ATOM	1308	OG1	THR	800	20.773	16.729	11.396	1.00	53.15	O
ATOM	1310	CG2	THR	800	22.696	16.813	9.968	1.00	53.33	C
ATOM	1311	C	THR	800	18.883	17.205	9.354	1.00	48.95	C
ATOM	1312	O	THR	800	18.345	18.013	10.125	1.00	55.00	O
ATOM	1313	N	PRO	801	18.170	16.238	8.740	1.00	47.30	N
ATOM	1314	CD	PRO	801	18.603	15.381	7.615	1.00	45.27	C
ATOM	1315	CA	PRO	801	16.733	16.068	9.000	1.00	42.31	C
ATOM	1316	CB	PRO	801	16.404	14.799	8.221	1.00	47.59	C
ATOM	1317	CG	PRO	801	17.285	14.951	7.007	1.00	46.66	C
ATOM	1318	C	PRO	801	16.353	15.955	10.476	1.00	38.64	C
ATOM	1319	O	PRO	801	15.193	16.130	10.835	1.00	40.23	O
ATOM	1320	N	GLN	802	17.351	15.682	11.310	1.00	41.68	N
ATOM	1322	CA	GLN	802	17.210	15.560	12.754	1.00	43.58	C
ATOM	1323	CB	GLN	802	18.338	14.684	13.311	1.00	46.98	C
ATOM	1324	CG	GLN	802	18.321	13.250	12.830	1.00	46.45	C
ATOM	1325	CD	GLN	802	18.685	13.116	11.373	1.00	48.73	C
ATOM	1326	OE1	GLN	802	19.827	13.413	10.968	1.00	53.22	O
ATOM	1327	NE2	GLN	802	17.727	12.666	10.566	1.00	43.12	N
ATOM	1330	C	GLN	802	17.275	16.959	13.403	1.00	48.44	C
ATOM	1331	O	GLN	802	16.505	17.266	14.329	1.00	49.81	O
ATOM	1332	N	GLU	803	18.218	17.790	12.950	1.00	41.48	N
ATOM	1334	CA	GLU	803	18.322	19.142	13.483	1.00	32.56	C
ATOM	1335	CB	GLU	803	19.485	19.869	12.879	1.00	27.56	C
ATOM	1336	CG	GLU	803	20.796	19.325	13.342	1.00	33.55	C
ATOM	1337	CD	GLU	803	21.903	19.778	12.436	1.00	40.34	C
ATOM	1338	OE1	GLU	803	21.618	20.023	11.249	1.00	39.58	O
ATOM	1339	OE2	GLU	803	23.057	19.915	12.882	1.00	46.91	O
ATOM	1340	C	GLU	803	17.034	19.841	13.133	1.00	34.21	C
ATOM	1341	O	GLU	803	16.456	20.543	13.951	1.00	39.30	O
ATOM	1342	N	PHE	804	16.541	19.584	11.932	1.00	32.10	N
ATOM	1344	CA	PHE	804	15.286	20.166	11.519	1.00	26.58	C
ATOM	1345	CB	PHE	804	14.872	19.663	10.142	1.00	24.46	C
ATOM	1346	CG	PHE	804	13.445	20.032	9.767	1.00	35.13	C
ATOM	1347	CD1	PHE	804	13.091	21.361	9.540	1.00	36.25	C
ATOM	1348	CD2	PHE	804	12.468	19.048	9.617	1.00	38.14	C
ATOM	1349	CE1	PHE	804	11.795	21.712	9.164	1.00	27.83	C
ATOM	1350	CE2	PHE	804	11.163	19.385	9.238	1.00	39.32	C
ATOM	1351	CZ	PHE	804	10.826	20.723	9.011	1.00	38.61	C
ATOM	1352	C	PHE	804	14.157	19.876	12.497	1.00	29.08	C
ATOM	1353	O	PHE	804	13.528	20.793	13.024	1.00	38.23	O
ATOM	1354	N	LEU	805	13.887	18.600	12.728	1.00	30.73	N
ATOM	1356	CA	LEU	805	12.784	18.215	13.586	1.00	28.43	C
ATOM	1357	CB	LEU	805	12.648	16.702	13.661	1.00	34.10	C
ATOM	1358	CG	LEU	805	12.000	16.079	12.423	1.00	43.20	C
ATOM	1359	CD1	LEU	805	12.046	14.617	12.600	1.00	36.94	C
ATOM	1360	CD2	LEU	805	10.549	16.523	12.252	1.00	44.97	C
ATOM	1361	C	LEU	805	12.880	18.799	14.946	1.00	26.10	C
ATOM	1362	O	LEU	805	11.881	19.243	15.493	1.00	34.14	O

FIG. 6 CONT'D

ATOM	1363	N	CYS	806	14.082	18.836	15.493	1.00 27.20	N
ATOM	1365	CA	CYS	806	14.250	19.396	16.831	1.00 39.83	C
ATOM	1366	CB	CYS	806	15.669	19.143	17.341	1.00 43.31	C
ATOM	1367	SG	CYS	806	16.021	17.398	17.526	0.50 37.47	S
ATOM	1368	C	CYS	806	13.904	20.894	16.843	1.00 41.37	C
ATOM	1369	O	CYS	806	13.145	21.367	17.704	1.00 38.83	O
ATOM	1370	N	MET	807	14.420	21.610	15.846	1.00 38.56	N
ATOM	1372	CA	MET	807	14.161	23.027	15.692	1.00 33.72	C
ATOM	1373	CB	MET	807	14.973	23.589	14.519	1.00 37.50	C
ATOM	1374	CG	MET	807	16.474	23.539	14.740	1.00 38.94	C
ATOM	1375	SD	MET	807	17.486	24.563	13.596	1.00 42.84	S
ATOM	1376	CE	MET	807	17.165	23.799	12.065	1.00 49.58	C
ATOM	1377	C	MET	807	12.662	23.301	15.488	1.00 31.70	C
ATOM	1378	O	MET	807	12.093	24.168	16.148	1.00 37.83	O
ATOM	1379	N	LYS	808	12.006	22.545	14.617	1.00 27.59	N
ATOM	1381	CA	LYS	808	10.597	22.787	14.378	1.00 27.15	C
ATOM	1382	CB	LYS	808	10.029	21.837	13.313	1.00 24.49	C
ATOM	1383	CG	LYS	808	8.598	22.158	12.811	1.00 23.62	C
ATOM	1384	CD	LYS	808	8.148	21.143	11.740	1.00 24.64	C
ATOM	1385	CE	LYS	808	7.157	20.101	12.280	1.00 29.39	C
ATOM	1386	NZ	LYS	808	5.683	20.529	12.198	1.00 36.92	N
ATOM	1390	C	LYS	808	9.841	22.681	15.686	1.00 29.83	C
ATOM	1391	O	LYS	808	8.954	23.486	15.952	1.00 35.67	O
ATOM	1392	N	ALA	809	10.220	21.727	16.530	1.00 32.53	N
ATOM	1394	CA	ALA	809	9.553	21.557	17.826	1.00 38.51	C
ATOM	1395	CB	ALA	809	10.029	20.295	18.501	1.00 25.72	C
ATOM	1396	C	ALA	809	9.786	22.766	18.749	1.00 43.27	C
ATOM	1397	O	ALA	809	8.844	23.305	19.346	1.00 43.55	O
ATOM	1398	N	LEU	810	11.042	23.193	18.836	1.00 41.18	N
ATOM	1400	CA	LEU	810	11.460	24.340	19.651	1.00 40.05	C
ATOM	1401	CB	LEU	810	12.961	24.534	19.502	1.00 39.64	C
ATOM	1402	CG	LEU	810	13.779	25.313	20.524	1.00 43.39	C
ATOM	1403	CD1	LEU	810	13.361	24.959	21.942	1.00 41.58	C
ATOM	1404	CD2	LEU	810	15.256	24.981	20.284	1.00 34.95	C
ATOM	1405	C	LEU	810	10.732	25.626	19.269	1.00 38.85	C
ATOM	1406	O	LEU	810	10.445	26.460	20.134	1.00 38.70	O
ATOM	1407	N	LEU	811	10.409	25.763	17.982	1.00 31.82	N
ATOM	1409	CA	LEU	811	9.683	26.923	17.489	1.00 34.47	C
ATOM	1410	CB	LEU	811	9.384	26.811	15.988	1.00 33.79	C
ATOM	1411	CG	LEU	811	10.309	27.474	14.973	1.00 28.95	C
ATOM	1412	CD1	LEU	811	9.523	27.595	13.709	1.00 30.30	C
ATOM	1413	CD2	LEU	811	10.767	28.875	15.444	1.00 20.35	C
ATOM	1414	C	LEU	811	8.359	27.093	18.200	1.00 35.94	C
ATOM	1415	O	LEU	811	7.918	28.219	18.435	1.00 47.05	O
ATOM	1416	N	LEU	812	7.713	25.978	18.527	1.00 31.68	N
ATOM	1418	CA	LEU	812	6.418	26.032	19.190	1.00 30.90	C
ATOM	1419	CB	LEU	812	5.934	24.622	19.511	1.00 29.23	C
ATOM	1420	CG	LEU	812	4.600	24.544	20.281	1.00 34.64	C
ATOM	1421	CD1	LEU	812	3.428	25.002	19.417	1.00 30.86	C
ATOM	1422	CD2	LEU	812	4.355	23.144	20.738	1.00 31.58	C
ATOM	1423	C	LEU	812	6.459	26.850	20.469	1.00 29.57	C
ATOM	1424	O	LEU	812	5.476	27.486	20.836	1.00 35.81	O
ATOM	1425	N	PHE	813	7.604	26.788	21.144	1.00 32.36	N
ATOM	1427	CA	PHE	813	7.862	27.480	22.405	1.00 36.84	C
ATOM	1428	CB	PHE	813	8.669	26.585	23.335	1.00 39.81	C
ATOM	1429	CG	PHE	813	8.119	25.242	23.454	1.00 42.06	C

FIG. 6 CONT'D

ATOM	1430	CD1	PHE	813	6.837	25.057	23.960	1.00	40.53	C
ATOM	1431	CD2	PHE	813	8.826	24.156	22.984	1.00	43.44	C
ATOM	1432	CE1	PHE	813	6.255	23.794	23.990	1.00	49.40	C
ATOM	1433	CE2	PHE	813	8.259	22.884	23.006	1.00	48.76	C
ATOM	1434	CZ	PHE	813	6.966	22.698	23.510	1.00	49.26	C
ATOM	1435	C	PHE	813	8.709	28.693	22.180	1.00	36.98	C
ATOM	1436	O	PHE	813	9.584	28.983	22.996	1.00	34.78	O
ATOM	1437	N	SER	814	8.488	29.380	21.071	1.00	39.85	N
ATOM	1439	CA	SER	814	9.284	30.547	20.748	1.00	40.33	C
ATOM	1440	CB	SER	814	9.938	30.364	19.374	1.00	45.33	C
ATOM	1441	OG	SER	814	11.096	29.544	19.469	1.00	51.73	O
ATOM	1443	C	SER	814	8.531	31.858	20.778	1.00	34.59	C
ATOM	1444	O	SER	814	9.125	32.897	20.612	1.00	39.81	O
ATOM	1445	N	ILE	815	7.242	31.838	21.040	1.00	38.17	N
ATOM	1447	CA	ILE	815	6.508	33.083	21.033	1.00	46.03	C
ATOM	1448	CB	ILE	815	5.937	33.329	19.597	1.00	49.44	C
ATOM	1449	CG2	ILE	815	5.401	32.041	18.971	1.00	50.44	C
ATOM	1450	CG1	ILE	815	4.943	34.477	19.593	1.00	50.62	C
ATOM	1451	CD1	ILE	815	5.406	35.592	18.748	1.00	55.65	C
ATOM	1452	C	ILE	815	5.456	33.076	22.149	1.00	46.20	C
ATOM	1453	O	ILE	815	4.526	32.260	22.112	1.00	45.64	O
ATOM	1454	N	ILE	816	5.645	33.950	23.152	1.00	47.67	N
ATOM	1456	CA	ILE	816	4.762	34.056	24.344	1.00	46.12	C
ATOM	1457	CB	ILE	816	5.446	33.417	25.609	1.00	50.07	C
ATOM	1458	CG2	ILE	816	5.819	31.970	25.326	1.00	52.85	C
ATOM	1459	CG1	ILE	816	6.701	34.194	26.018	1.00	49.09	C
ATOM	1460	CD1	ILE	816	7.442	33.578	27.204	1.00	37.43	C
ATOM	1461	C	ILE	816	4.302	35.482	24.731	1.00	42.20	C
ATOM	1462	O	ILE	816	5.002	36.460	24.436	1.00	43.23	O
ATOM	1463	N	PRO	817	3.123	35.618	25.402	1.00	37.07	N
ATOM	1464	CD	PRO	817	2.186	34.579	25.855	1.00	33.43	C
ATOM	1465	CA	PRO	817	2.619	36.933	25.811	1.00	40.94	C
ATOM	1466	CB	PRO	817	1.396	36.581	26.662	1.00	27.66	C
ATOM	1467	CG	PRO	817	0.902	35.368	26.063	1.00	28.99	C
ATOM	1468	C	PRO	817	3.702	37.599	26.659	1.00	49.75	C
ATOM	1469	O	PRO	817	4.595	36.891	27.163	1.00	47.60	O
ATOM	1470	N	VAL	818	3.663	38.933	26.798	1.00	57.41	N
ATOM	1472	CA	VAL	818	4.690	39.631	27.592	1.00	58.97	C
ATOM	1473	CB	VAL	818	4.893	41.127	27.206	1.00	54.46	C
ATOM	1474	CG1	VAL	818	5.738	41.211	25.950	1.00	49.94	C
ATOM	1475	CG2	VAL	818	3.575	41.824	27.009	1.00	53.66	C
ATOM	1476	C	VAL	818	4.728	39.410	29.124	1.00	59.31	C
ATOM	1477	O	VAL	818	5.801	39.574	29.720	1.00	63.79	O
ATOM	1478	N	ASP	819	3.607	39.061	29.769	1.00	56.35	N
ATOM	1480	CA	ASP	819	3.654	38.741	31.212	1.00	61.78	C
ATOM	1481	CB	ASP	819	2.270	38.746	31.869	1.00	60.71	C
ATOM	1482	CG	ASP	819	1.174	39.031	30.888	1.00	71.79	C
ATOM	1483	OD1	ASP	819	0.947	40.218	30.600	1.00	78.23	O
ATOM	1484	OD2	ASP	819	0.577	38.069	30.373	1.00	78.87	O
ATOM	1485	C	ASP	819	4.167	37.302	31.212	1.00	63.93	C
ATOM	1486	O	ASP	819	5.322	36.998	31.566	1.00	69.29	O
ATOM	1487	N	GLY	820	3.296	36.419	30.758	1.00	57.92	N
ATOM	1489	CA	GLY	820	3.652	35.034	30.672	1.00	46.58	C
ATOM	1490	C	GLY	820	2.369	34.304	30.440	1.00	45.74	C
ATOM	1491	O	GLY	820	1.293	34.894	30.200	1.00	40.14	O
ATOM	1492	N	LEU	821	2.497	32.995	30.500	1.00	46.98	N

FIG. 6 CONT'D

ATOM	1494	CA	LEU	821	1.378	32.105	30.327	1.00 47.93	C
ATOM	1495	CB	LEU	821	1.905	30.808	29.708	1.00 54.39	C
ATOM	1496	CG	LEU	821	2.560	31.017	28.336	1.00 50.67	C
ATOM	1497	CD1	LEU	821	3.858	30.259	28.235	1.00 43.32	C
ATOM	1498	CD2	LEU	821	1.602	30.622	27.240	1.00 46.90	C
ATOM	1499	C	LEU	821	0.787	31.902	31.733	1.00 47.05	C
ATOM	1500	O	LEU	821	1.456	32.188	32.737	1.00 45.88	O
ATOM	1501	N	LYS	822	-0.437	31.393	31.820	1.00 48.17	N
ATOM	1503	CA	LYS	822	-1.103	31.181	33.105	1.00 52.88	C
ATOM	1504	CB	LYS	822	-2.609	30.951	32.880	1.00 56.87	C
ATOM	1505	CG	LYS	822	-3.321	32.193	32.288	1.00 65.23	C
ATOM	1506	CD	LYS	822	-4.729	31.923	31.719	1.00 63.38	C
ATOM	1507	CE	LYS	822	-5.371	33.194	31.088	1.00 65.28	C
ATOM	1508	NZ	LYS	822	-4.534	33.875	30.032	1.00 59.84	N
ATOM	1512	C	LYS	822	-0.449	30.065	33.935	1.00 59.84	C
ATOM	1513	O	LYS	822	-1.111	29.361	34.709	1.00 62.81	O
ATOM	1514	N	ASN	823	0.862	29.930	33.744	1.00 62.47	N
ATOM	1516	CA	ASN	823	1.739	28.988	34.419	1.00 60.37	C
ATOM	1517	CB	ASN	823	1.138	27.611	34.544	1.00 65.57	C
ATOM	1518	CG	ASN	823	2.094	26.649	35.178	1.00 75.73	C
ATOM	1519	OD1	ASN	823	3.101	27.051	35.811	1.00 68.88	O
ATOM	1520	ND2	ASN	823	1.830	25.367	34.986	1.00 81.03	N
ATOM	1523	C	ASN	823	3.025	28.904	33.616	1.00 58.03	C
ATOM	1524	O	ASN	823	3.364	27.879	33.017	1.00 50.60	O
ATOM	1525	N	GLN	824	3.743	30.012	33.631	1.00 59.10	N
ATOM	1527	CA	GLN	824	4.993	30.158	32.914	1.00 56.38	C
ATOM	1528	CB	GLN	824	5.485	31.592	33.129	1.00 56.68	C
ATOM	1529	CG	GLN	824	6.761	31.972	32.412	1.00 54.92	C
ATOM	1530	CD	GLN	824	6.532	32.329	30.976	1.00 59.81	C
ATOM	1531	OE1	GLN	824	5.462	32.833	30.602	1.00 57.91	O
ATOM	1532	NE2	GLN	824	7.533	32.078	30.150	1.00 62.36	N
ATOM	1535	C	GLN	824	6.069	29.145	33.329	1.00 54.52	C
ATOM	1536	O	GLN	824	6.826	28.677	32.483	1.00 53.91	O
ATOM	1537	N	LYS	825	6.099	28.777	34.613	1.00 55.18	N
ATOM	1539	CA	LYS	825	7.098	27.841	35.160	1.00 53.31	C
ATOM	1540	CB	LYS	825	6.769	27.515	36.626	1.00 57.76	C
ATOM	1541	CG	LYS	825	7.128	28.634	37.617	1.00 64.19	C
ATOM	1542	CD	LYS	825	6.432	28.463	38.979	1.00 77.45	C
ATOM	1543	CE	LYS	825	7.122	29.254	40.125	1.00 86.97	C
ATOM	1544	NZ	LYS	825	7.186	30.763	40.023	1.00 89.42	N
ATOM	1548	C	LYS	825	7.351	26.550	34.357	1.00 46.62	C
ATOM	1549	O	LYS	825	8.497	26.236	34.015	1.00 40.85	O
ATOM	1550	N	PHE	826	6.285	25.811	34.053	1.00 46.35	N
ATOM	1552	CA	PHE	826	6.399	24.562	33.288	1.00 47.42	C
ATOM	1553	CB	PHE	826	5.063	23.774	33.273	1.00 43.87	C
ATOM	1554	CG	PHE	826	4.588	23.295	34.653	1.00 56.48	C
ATOM	1555	CD1	PHE	826	5.443	23.288	35.770	1.00 62.15	C
ATOM	1556	CD2	PHE	826	3.273	22.832	34.831	1.00 60.89	C
ATOM	1557	CE1	PHE	826	4.994	22.827	37.040	1.00 53.25	C
ATOM	1558	CE2	PHE	826	2.813	22.367	36.097	1.00 53.93	C
ATOM	1559	CZ	PHE	826	3.681	22.368	37.193	1.00 51.47	C
ATOM	1560	C	PHE	826	6.892	24.863	31.853	1.00 48.67	C
ATOM	1561	O	PHE	826	7.847	24.243	31.395	1.00 48.05	O
ATOM	1562	N	PHE	827	6.272	25.835	31.168	1.00 44.70	N
ATOM	1564	CA	PHE	827	6.670	26.234	29.800	1.00 40.53	C
ATOM	1565	CB	PHE	827	5.964	27.558	29.375	1.00 35.40	C

FIG. 6 CONT'D

ATOM	1566	CG	PHE	827	6.497	28.177	28.070	1.00 31.04	C
ATOM	1567	CD1	PHE	827	5.742	28.125	26.900	1.00 34.40	C
ATOM	1568	CD2	PHE	827	7.750	28.793	28.018	1.00 32.73	C
ATOM	1569	CE1	PHE	827	6.225	28.664	25.705	1.00 26.27	C
ATOM	1570	CE2	PHE	827	8.239	29.331	26.834	1.00 34.03	C
ATOM	1571	CZ	PHE	827	7.472	29.265	25.676	1.00 30.82	C
ATOM	1572	C	PHE	827	8.181	26.414	29.746	1.00 37.37	C
ATOM	1573	O	PHE	827	8.848	25.934	28.835	1.00 35.40	O
ATOM	1574	N	ASP	828	8.705	27.105	30.745	1.00 42.94	N
ATOM	1576	CA	ASP	828	10.120	27.388	30.829	1.00 49.10	C
ATOM	1577	CB	ASP	828	10.371	28.459	31.899	1.00 53.78	C
ATOM	1578	CG	ASP	828	9.730	29.810	31.539	1.00 65.91	C
ATOM	1579	OD1	ASP	828	9.610	30.121	30.329	1.00 69.82	O
ATOM	1580	OD2	ASP	828	9.357	30.576	32.461	1.00 63.94	O
ATOM	1581	C	ASP	828	10.933	26.130	31.071	1.00 49.16	C
ATOM	1582	O	ASP	828	12.107	26.056	30.681	1.00 48.64	O
ATOM	1583	N	GLU	829	10.313	25.138	31.703	1.00 49.55	N
ATOM	1585	CA	GLU	829	10.997	23.875	31.941	1.00 49.00	C
ATOM	1586	CB	GLU	829	10.350	23.073	33.076	1.00 61.68	C
ATOM	1587	CG	GLU	829	11.366	22.268	33.925	1.00 81.07	C
ATOM	1588	CD	GLU	829	10.939	20.814	34.222	1.00 92.42	C
ATOM	1589	OE1	GLU	829	11.619	19.881	33.727	1.00 91.99	O
ATOM	1590	OE2	GLU	829	9.952	20.603	34.969	1.00 97.07	O
ATOM	1591	C	GLU	829	10.952	23.103	30.622	1.00 37.58	C
ATOM	1592	O	GLU	829	11.969	22.573	30.177	1.00 35.86	O
ATOM	1593	N	LEU	830	9.794	23.102	29.962	1.00 33.30	N
ATOM	1595	CA	LEU	830	9.626	22.436	28.661	1.00 37.63	C
ATOM	1596	CB	LEU	830	8.240	22.701	28.083	1.00 30.37	C
ATOM	1597	CG	LEU	830	7.257	21.551	28.118	1.00 39.95	C
ATOM	1598	CD1	LEU	830	6.108	21.877	27.212	1.00 34.14	C
ATOM	1599	CD2	LEU	830	7.951	20.268	27.671	1.00 49.69	C
ATOM	1600	C	LEU	830	10.621	23.003	27.673	1.00 41.33	C
ATOM	1601	O	LEU	830	11.366	22.261	27.031	1.00 46.84	O
ATOM	1602	N	ARG	831	10.621	24.333	27.566	1.00 44.13	N
ATOM	1604	CA	ARG	831	11.504	25.048	26.658	1.00 40.24	C
ATOM	1605	CB	ARG	831	11.285	26.566	26.765	1.00 34.87	C
ATOM	1606	CG	ARG	831	12.179	27.322	25.816	1.00 34.44	C
ATOM	1607	CD	ARG	831	11.915	28.804	25.731	1.00 38.71	C
ATOM	1608	NE	ARG	831	13.020	29.423	25.006	1.00 39.34	N
ATOM	1610	CZ	ARG	831	13.073	29.573	23.682	1.00 44.99	C
ATOM	1611	NH1	ARG	831	12.060	29.164	22.926	1.00 40.07	N
ATOM	1614	NH2	ARG	831	14.178	30.050	23.104	1.00 41.88	N
ATOM	1617	C	ARG	831	12.977	24.673	26.862	1.00 37.21	C
ATOM	1618	O	ARG	831	13.690	24.354	25.901	1.00 37.75	O
ATOM	1619	N	MET	832	13.411	24.625	28.116	1.00 38.65	N
ATOM	1621	CA	MET	832	14.799	24.281	28.440	1.00 43.09	C
ATOM	1622	CB	MET	832	15.065	24.409	29.941	1.00 41.77	C
ATOM	1623	CG	MET	832	16.486	23.967	30.274	1.00 50.47	C
ATOM	1624	SD	MET	832	16.856	23.608	31.997	1.00 61.59	S
ATOM	1625	CE	MET	832	15.233	23.187	32.715	1.00 51.34	C
ATOM	1626	C	MET	832	15.239	22.880	27.996	1.00 44.84	C
ATOM	1627	O	MET	832	16.400	22.662	27.602	1.00 43.33	O
ATOM	1628	N	ASN	833	14.339	21.914	28.141	1.00 46.14	N
ATOM	1630	CA	ASN	833	14.661	20.552	27.754	1.00 44.12	C
ATOM	1631	CB	ASN	833	13.689	19.580	28.379	1.00 47.22	C
ATOM	1632	CG	ASN	833	14.098	19.202	29.782	1.00 44.35	C

FIG. 6 CONT'D

ATOM	1633	OD1	ASN	833	15.262	18.849	30.041	1.00	53.06	O
ATOM	1634	ND2	ASN	833	13.161	19.299	30.705	1.00	42.24	N
ATOM	1637	C	ASN	833	14.756	20.387	26.255	1.00	40.57	C
ATOM	1638	O	ASN	833	15.670	19.729	25.766	1.00	45.06	O
ATOM	1639	N	TYR	834	13.866	21.048	25.523	1.00	35.70	N
ATOM	1641	CA	TYR	834	13.923	21.006	24.074	1.00	36.60	C
ATOM	1642	CB	TYR	834	12.723	21.729	23.473	1.00	33.03	C
ATOM	1643	CG	TYR	834	11.480	20.849	23.446	1.00	39.21	C
ATOM	1644	CD1	TYR	834	11.085	20.196	22.274	1.00	38.14	C
ATOM	1645	CE1	TYR	834	9.959	19.337	22.255	1.00	42.60	C
ATOM	1646	CD2	TYR	834	10.724	20.630	24.597	1.00	41.70	C
ATOM	1647	CE2	TYR	834	9.598	19.774	24.587	1.00	44.38	C
ATOM	1648	CZ	TYR	834	9.229	19.132	23.416	1.00	42.12	C
ATOM	1649	OH	TYR	834	8.164	18.264	23.404	1.00	38.82	O
ATOM	1651	C	TYR	834	15.260	21.582	23.589	1.00	35.58	C
ATOM	1652	O	TYR	834	15.891	21.044	22.670	1.00	39.23	O
ATOM	1653	N	ILE	835	15.754	22.607	24.275	1.00	37.68	N
ATOM	1655	CA	ILE	835	17.042	23.197	23.901	1.00	42.31	C
ATOM	1656	CB	ILE	835	17.408	24.417	24.782	1.00	37.10	C
ATOM	1657	CG2	ILE	835	18.832	24.912	24.457	1.00	29.58	C
ATOM	1658	CG1	ILE	835	16.357	25.512	24.558	1.00	41.30	C
ATOM	1659	CD1	ILE	835	16.610	26.802	25.286	1.00	39.55	C
ATOM	1660	C	ILE	835	18.103	22.133	24.060	1.00	42.75	C
ATOM	1661	O	ILE	835	18.995	21.997	23.217	1.00	45.95	O
ATOM	1662	N	LYS	836	17.980	21.373	25.144	1.00	44.22	N
ATOM	1664	CA	LYS	836	18.925	20.313	25.442	1.00	44.77	C
ATOM	1665	CB	LYS	836	18.655	19.694	26.813	1.00	46.26	C
ATOM	1666	CG	LYS	836	19.116	20.512	28.011	1.00	49.87	C
ATOM	1667	CD	LYS	836	18.609	19.834	29.274	0.00	50.55	C
ATOM	1668	CE	LYS	836	19.311	20.321	30.524	0.00	51.77	C
ATOM	1669	NZ	LYS	836	18.709	19.697	31.735	0.00	52.70	N
ATOM	1673	C	LYS	836	18.846	19.252	24.363	1.00	41.28	C
ATOM	1674	O	LYS	836	19.866	18.780	23.914	1.00	46.84	O
ATOM	1675	N	GLU	837	17.655	18.928	23.883	1.00	40.62	N
ATOM	1677	CA	GLU	837	17.543	17.899	22.851	1.00	44.21	C
ATOM	1678	CB	GLU	837	16.077	17.573	22.516	1.00	43.88	C
ATOM	1679	CG	GLU	837	15.226	17.032	23.675	1.00	44.03	C
ATOM	1680	CD	GLU	837	15.937	15.978	24.534	1.00	50.34	C
ATOM	1681	OE1	GLU	837	16.915	15.332	24.076	1.00	45.21	O
ATOM	1682	OE2	GLU	837	15.512	15.804	25.696	1.00	56.07	O
ATOM	1683	C	GLU	837	18.253	18.344	21.603	1.00	43.91	C
ATOM	1684	O	GLU	837	18.902	17.549	20.922	1.00	49.11	O
ATOM	1685	N	LEU	838	18.113	19.627	21.305	1.00	44.87	N
ATOM	1687	CA	LEU	838	18.739	20.218	20.139	1.00	43.87	C
ATOM	1688	CB	LEU	838	18.324	21.675	20.019	1.00	42.66	C
ATOM	1689	CG	LEU	838	19.051	22.463	18.932	1.00	44.98	C
ATOM	1690	CD1	LEU	838	18.810	21.814	17.567	1.00	39.69	C
ATOM	1691	CD2	LEU	838	18.571	23.909	18.964	1.00	37.64	C
ATOM	1692	C	LEU	838	20.244	20.120	20.285	1.00	42.53	C
ATOM	1693	O	LEU	838	20.949	19.835	19.332	1.00	42.95	O
ATOM	1694	N	ASP	839	20.713	20.346	21.501	1.00	44.58	N
ATOM	1696	CA	ASP	839	22.129	20.286	21.844	1.00	52.02	C
ATOM	1697	CB	ASP	839	22.262	20.760	23.305	1.00	59.66	C
ATOM	1698	CG	ASP	839	23.673	21.234	23.674	1.00	66.70	C
ATOM	1699	OD1	ASP	839	24.584	21.284	22.812	1.00	65.99	O
ATOM	1700	OD2	ASP	839	23.850	21.598	24.860	1.00	68.25	O

FIG. 6 CONT'D

ATOM	1701	C	ASP	839	22.630	18.829	21.696	1.00	57.30	C
ATOM	1702	O	ASP	839	23.750	18.569	21.224	1.00	54.16	O
ATOM	1703	N	ARG	840	21.768	17.884	22.081	1.00	62.29	N
ATOM	1705	CA	ARG	840	22.065	16.453	22.022	1.00	62.05	C
ATOM	1706	CB	ARG	840	20.927	15.623	22.643	1.00	61.97	C
ATOM	1707	CG	ARG	840	21.035	14.114	22.407	1.00	62.90	C
ATOM	1708	CD	ARG	840	20.219	13.320	23.422	1.00	62.88	C
ATOM	1709	NE	ARG	840	20.676	13.542	24.799	1.00	67.96	N
ATOM	1711	CZ	ARG	840	19.875	13.676	25.861	1.00	65.20	C
ATOM	1712	NH1	ARG	840	18.550	13.618	25.718	1.00	60.29	N
ATOM	1715	NH2	ARG	840	20.404	13.889	27.066	1.00	61.82	N
ATOM	1718	C	ARG	840	22.280	16.022	20.591	1.00	60.23	C
ATOM	1719	O	ARG	840	23.331	15.468	20.268	1.00	57.37	O
ATOM	1720	N	ILE	841	21.298	16.311	19.739	1.00	57.25	N
ATOM	1722	CA	ILE	841	21.344	15.956	18.325	1.00	64.29	C
ATOM	1723	CB	ILE	841	19.998	16.261	17.674	1.00	66.05	C
ATOM	1724	CG2	ILE	841	18.887	15.730	18.567	1.00	69.45	C
ATOM	1725	CG1	ILE	841	19.813	17.765	17.505	1.00	60.52	C
ATOM	1726	CD1	ILE	841	18.835	18.115	16.439	1.00	55.24	C
ATOM	1727	C	ILE	841	22.494	16.602	17.508	1.00	71.86	C
ATOM	1728	O	ILE	841	22.706	16.276	16.327	1.00	78.18	O
ATOM	1729	N	ILE	842	23.210	17.541	18.127	1.00	74.71	N
ATOM	1731	CA	ILE	842	24.354	18.208	17.489	1.00	72.84	C
ATOM	1732	CB	ILE	842	24.507	19.684	17.990	1.00	62.10	C
ATOM	1733	CG2	ILE	842	25.769	20.303	17.439	1.00	59.08	C
ATOM	1734	CG1	ILE	842	23.312	20.522	17.569	1.00	54.67	C
ATOM	1735	CD1	ILE	842	23.101	20.519	16.109	1.00	56.78	C
ATOM	1736	C	ILE	842	25.643	17.430	17.845	1.00	76.76	C
ATOM	1737	O	ILE	842	26.431	17.080	16.952	1.00	76.88	O
ATOM	1738	N	ALA	843	25.819	17.166	19.152	1.00	82.38	N
ATOM	1740	CA	ALA	843	26.979	16.461	19.733	1.00	81.09	C
ATOM	1741	CB	ALA	843	27.076	16.768	21.247	1.00	73.81	C
ATOM	1742	C	ALA	843	26.960	14.955	19.524	1.00	79.83	C
ATOM	1743	O	ALA	843	27.924	14.260	19.838	1.00	79.34	O
ATOM	1744	N	CYS	844	25.872	14.469	18.947	1.00	80.33	N
ATOM	1746	CA	CYS	844	25.657	13.052	18.721	1.00	80.34	C
ATOM	1747	C	CYS	844	25.771	12.645	17.215	1.00	84.98	C
ATOM	1748	O	CYS	844	25.056	11.750	16.759	1.00	90.65	O
ATOM	1749	CB	CYS	844	24.269	12.717	19.315	1.00	80.98	N
ATOM	1750	SG	CYS	844	24.002	11.110	20.120	1.00	93.38	S
ATOM	1751	N	LYS	845	26.665	13.302	16.460	1.00	86.19	N
ATOM	1753	CA	LYS	845	26.917	13.002	15.026	1.00	83.63	C
ATOM	1754	CB	LYS	845	26.063	13.874	14.087	1.00	72.76	C
ATOM	1755	CG	LYS	845	24.727	13.263	13.735	1.00	66.51	C
ATOM	1756	CD	LYS	845	23.998	14.104	12.702	0.00	63.58	C
ATOM	1757	CE	LYS	845	24.644	14.005	11.326	0.00	60.54	C
ATOM	1758	NZ	LYS	845	23.795	13.251	10.351	0.00	57.84	N
ATOM	1762	C	LYS	845	28.420	13.101	14.620	1.00	90.32	C
ATOM	1763	O	LYS	845	29.110	12.079	14.517	1.00	87.60	O
ATOM	1764	N	ARG	846	28.929	14.316	14.384	1.00	97.68	N
ATOM	1766	CA	ARG	846	30.336	14.489	13.998	1.00	99.68	C
ATOM	1767	CB	ARG	846	30.442	15.246	12.671	1.00	94.46	C
ATOM	1768	CG	ARG	846	31.702	14.917	11.839	1.00	92.16	C
ATOM	1769	CD	ARG	846	31.538	13.643	10.999	1.00	87.99	C
ATOM	1770	NE	ARG	846	32.671	12.718	11.128	1.00	86.09	N
ATOM	1772	CZ	ARG	846	32.667	11.463	10.675	1.00	85.82	C

FIG. 6 CONT'D

ATOM	1773	NH1	ARG	846	31.583	10.985	10.058	1.00 79.74	N
ATOM	1776	NH2	ARG	846	33.720	10.666	10.891	1.00 82.90	N
ATOM	1779	C	ARG	846	31.289	15.076	15.097	1.00104.16	C
ATOM	1780	O	ARG	846	31.315	14.556	16.229	1.00101.78	O
ATOM	1781	N	LYS	847	32.040	16.139	14.736	1.00109.20	N
ATOM	1783	CA	LYS	847	33.061	16.820	15.585	1.00108.66	C
ATOM	1784	CB	LYS	847	33.760	17.897	14.758	0.00 98.30	C
ATOM	1785	CG	LYS	847	34.514	17.383	13.563	0.00 85.34	C
ATOM	1786	CD	LYS	847	35.150	18.542	12.840	0.00 73.33	C
ATOM	1787	CE	LYS	847	35.928	18.073	11.641	0.00 64.16	C
ATOM	1788	NZ	LYS	847	36.604	19.219	10.996	0.00 56.55	N
ATOM	1792	C	LYS	847	32.769	17.424	16.961	1.00113.81	C
ATOM	1793	O	LYS	847	31.596	17.569	17.368	1.00118.99	O
ATOM	1794	N	ASN	848	33.860	17.821	17.636	1.00115.89	N
ATOM	1796	CA	ASN	848	33.904	18.449	18.991	1.00116.39	C
ATOM	1797	CB	ASN	848	33.392	17.448	20.089	1.00106.55	C
ATOM	1798	CG	ASN	848	33.984	16.032	19.955	1.00 99.70	C
ATOM	1799	OD1	ASN	848	35.078	15.825	19.426	1.00 96.25	O
ATOM	1800	ND2	ASN	848	33.240	15.046	20.457	1.00 89.90	N
ATOM	1803	C	ASN	848	35.379	18.906	19.266	1.00119.41	C
ATOM	1804	O	ASN	848	36.305	18.286	18.735	1.00122.42	O
ATOM	1805	N	PRO	849	35.622	20.019	20.031	1.00119.93	N
ATOM	1806	CD	PRO	849	37.039	20.160	20.430	1.00120.61	C
ATOM	1807	CA	PRO	849	34.808	21.031	20.742	1.00119.46	C
ATOM	1808	CB	PRO	849	35.725	21.422	21.914	1.00118.16	C
ATOM	1809	CG	PRO	849	37.063	21.454	21.259	1.00118.96	C
ATOM	1810	C	PRO	849	34.292	22.298	20.008	1.00118.74	C
ATOM	1811	O	PRO	849	33.082	22.562	20.025	1.00121.98	O
ATOM	1812	N	THR	850	35.178	23.098	19.399	1.00113.94	N
ATOM	1814	CA	THR	850	34.738	24.330	18.701	1.00107.06	C
ATOM	1815	CB	THR	850	35.931	25.182	18.134	1.00105.27	C
ATOM	1816	OG1	THR	850	36.538	24.500	17.025	1.00104.75	O
ATOM	1818	CG2	THR	850	36.976	25.482	19.222	1.00 99.79	C
ATOM	1819	C	THR	850	33.693	24.100	17.584	1.00103.74	C
ATOM	1820	O	THR	850	32.820	24.944	17.372	1.00104.75	O
ATOM	1821	N	SER	851	33.788	22.949	16.909	1.00 98.29	N
ATOM	1823	CA	SER	851	32.885	22.562	15.810	1.00 93.63	C
ATOM	1824	CB	SER	851	33.319	21.185	15.262	1.00 93.65	C
ATOM	1825	OG	SER	851	32.729	20.888	14.012	1.00 96.10	O
ATOM	1827	C	SER	851	31.374	22.559	16.173	1.00 89.97	C
ATOM	1828	O	SER	851	30.553	23.123	15.429	1.00 85.73	O
ATOM	1829	N	CYS	852	31.000	21.964	17.311	1.00 87.36	N
ATOM	1831	CA	CYS	852	29.587	21.932	17.706	1.00 85.60	C
ATOM	1832	CB	CYS	852	29.260	20.605	18.409	1.00 85.66	C
ATOM	1833	SG	CYS	852	29.511	20.548	20.196	1.00 92.38	S
ATOM	1834	C	CYS	852	29.128	23.167	18.541	1.00 85.71	C
ATOM	1835	O	CYS	852	27.929	23.468	18.592	1.00 81.46	O
ATOM	1836	N	SER	853	30.071	23.873	19.184	1.00 88.63	N
ATOM	1838	CA	SER	853	29.760	25.085	19.970	1.00 85.42	C
ATOM	1839	CB	SER	853	31.015	25.615	20.702	1.00 83.41	C
ATOM	1840	OG	SER	853	31.524	24.733	21.692	1.00 75.95	O
ATOM	1842	C	SER	853	29.261	26.147	18.970	1.00 81.80	C
ATOM	1843	O	SER	853	28.320	26.914	19.260	1.00 75.88	O
ATOM	1844	N	ARG	854	29.929	26.190	17.806	1.00 77.44	N
ATOM	1846	CA	ARG	854	29.586	27.108	16.721	1.00 75.23	C
ATOM	1847	CB	ARG	854	30.803	27.423	15.831	1.00 83.31	C

FIG. 6 CONT'D

ATOM	1848	CG	ARG	854	31.492	26.211	15.215	1.00 95.75	C
ATOM	1849	CD	ARG	854	32.915	26.540	14.706	1.00105.49	C
ATOM	1850	NE	ARG	854	32.927	27.070	13.344	1.00111.61	N
ATOM	1852	CZ	ARG	854	33.255	28.318	13.014	1.00107.74	C
ATOM	1853	NH1	ARG	854	33.614	29.182	13.963	1.00108.73	N
ATOM	1856	NH2	ARG	854	33.171	28.704	11.740	1.00100.08	N
ATOM	1859	C	ARG	854	28.428	26.555	15.903	1.00 68.44	C
ATOM	1860	O	ARG	854	27.614	27.325	15.381	1.00 64.21	O
ATOM	1861	N	ARG	855	28.341	25.228	15.801	1.00 62.47	N
ATOM	1863	CA	ARG	855	27.229	24.606	15.087	1.00 56.87	C
ATOM	1864	CB	ARG	855	27.423	23.085	14.974	1.00 53.03	C
ATOM	1865	CG	ARG	855	26.247	22.321	14.341	1.00 51.39	C
ATOM	1866	CD	ARG	855	25.983	22.707	12.891	1.00 55.10	C
ATOM	1867	NE	ARG	855	24.943	21.899	12.233	1.00 54.36	N
ATOM	1869	CZ	ARG	855	24.745	21.858	10.911	1.00 55.00	C
ATOM	1870	NH1	ARG	855	25.517	22.579	10.110	1.00 52.83	N
ATOM	1873	NH2	ARG	855	23.796	21.094	10.384	1.00 48.85	N
ATOM	1876	C	ARG	855	25.922	24.945	15.831	1.00 55.34	C
ATOM	1877	O	ARG	855	24.861	25.054	15.206	1.00 61.05	O
ATOM	1878	N	PHE	856	26.003	25.152	17.152	1.00 52.54	N
ATOM	1880	CA	PHE	856	24.817	25.508	17.962	1.00 49.53	C
ATOM	1881	CB	PHE	856	25.066	25.270	19.457	1.00 46.16	C
ATOM	1882	CG	PHE	856	23.852	25.527	20.319	1.00 46.93	C
ATOM	1883	CD1	PHE	856	22.699	24.751	20.170	1.00 47.04	C
ATOM	1884	CD2	PHE	856	23.845	26.549	21.259	1.00 41.32	C
ATOM	1885	CE1	PHE	856	21.547	24.986	20.949	1.00 46.91	C
ATOM	1886	CE2	PHE	856	22.711	26.785	22.033	1.00 45.75	C
ATOM	1887	CZ	PHE	856	21.553	25.999	21.877	1.00 42.35	C
ATOM	1888	C	PHE	856	24.438	26.974	17.738	1.00 48.70	C
ATOM	1889	O	PHE	856	23.254	27.326	17.597	1.00 45.42	O
ATOM	1890	N	TYR	857	25.461	27.822	17.725	1.00 47.67	N
ATOM	1892	CA	TYR	857	25.283	29.238	17.487	1.00 47.32	C
ATOM	1893	CB	TYR	857	26.667	29.901	17.407	1.00 50.61	C
ATOM	1894	CG	TYR	857	26.684	31.282	16.807	1.00 54.67	C
ATOM	1895	CD1	TYR	857	26.450	32.422	17.593	1.00 59.56	C
ATOM	1896	CE1	TYR	857	26.469	33.719	17.022	1.00 58.68	C
ATOM	1897	CD2	TYR	857	26.935	31.454	15.442	1.00 54.77	C
ATOM	1898	CE2	TYR	857	26.953	32.728	14.860	1.00 58.39	C
ATOM	1899	CZ	TYR	857	26.720	33.855	15.647	1.00 61.97	C
ATOM	1900	OH	TYR	857	26.725	35.091	15.035	1.00 56.70	O
ATOM	1902	C	TYR	857	24.503	29.373	16.181	1.00 44.87	C
ATOM	1903	O	TYR	857	23.404	29.945	16.159	1.00 42.27	O
ATOM	1904	N	GLN	858	25.006	28.706	15.141	1.00 43.56	N
ATOM	1906	CA	GLN	858	24.400	28.744	13.803	1.00 42.92	C
ATOM	1907	CB	GLN	858	25.112	27.795	12.859	1.00 38.18	C
ATOM	1908	CG	GLN	858	26.563	28.061	12.645	1.00 41.30	C
ATOM	1909	CD	GLN	858	27.216	26.990	11.788	1.00 48.05	C
ATOM	1910	OE1	GLN	858	28.399	27.051	11.521	1.00 60.25	O
ATOM	1911	NE2	GLN	858	26.446	25.995	11.369	1.00 53.15	N
ATOM	1914	C	GLN	858	22.927	28.400	13.731	1.00 43.62	C
ATOM	1915	O	GLN	858	22.173	29.017	12.988	1.00 47.41	O
ATOM	1916	N	LEU	859	22.523	27.372	14.452	1.00 46.85	N
ATOM	1918	CA	LEU	859	21.136	26.956	14.407	1.00 44.50	C
ATOM	1919	CB	LEU	859	20.998	25.529	14.919	1.00 49.03	C
ATOM	1920	CG	LEU	859	21.571	24.412	14.044	1.00 51.91	C
ATOM	1921	CD1	LEU	859	21.563	23.090	14.809	1.00 49.78	C

FIG. 6 CONT'D

ATOM	1922	CD2	LEU	859	20.736	24.301	12.793	1.00	54.19	C
ATOM	1923	C	LEU	859	20.226	27.884	15.180	1.00	41.57	C
ATOM	1924	O	LEU	859	19.091	28.129	14.764	1.00	41.55	O
ATOM	1925	N	THR	860	20.712	28.393	16.307	1.00	36.22	N
ATOM	1927	CA	THR	860	19.910	29.300	17.111	1.00	36.58	C
ATOM	1928	CB	THR	860	20.557	29.532	18.474	1.00	35.81	C
ATOM	1929	OG1	THR	860	21.942	29.877	18.304	1.00	38.10	O
ATOM	1931	CG2	THR	860	20.445	28.256	19.302	1.00	33.36	C
ATOM	1932	C	THR	860	19.694	30.592	16.322	1.00	39.98	C
ATOM	1933	O	THR	860	18.600	31.177	16.351	1.00	41.71	O
ATOM	1934	N	LYS	861	20.718	30.998	15.564	1.00	35.42	N
ATOM	1936	CA	LYS	861	20.598	32.178	14.715	1.00	38.56	C
ATOM	1937	CB	LYS	861	21.932	32.530	14.076	1.00	35.42	C
ATOM	1938	CG	LYS	861	22.807	33.422	14.941	1.00	48.32	C
ATOM	1939	CD	LYS	861	22.394	34.906	14.850	1.00	56.04	C
ATOM	1940	CE	LYS	861	23.270	35.776	15.755	1.00	60.56	C
ATOM	1941	NZ	LYS	861	22.863	37.205	15.751	1.00	65.17	N
ATOM	1945	C	LYS	861	19.556	31.871	13.639	1.00	44.29	C
ATOM	1946	O	LYS	861	18.669	32.682	13.358	1.00	45.57	O
ATOM	1947	N	LEU	862	19.644	30.667	13.075	1.00	46.55	N
ATOM	1949	CA	LEU	862	18.690	30.228	12.069	1.00	39.38	C
ATOM	1950	CB	LEU	862	19.009	28.808	11.607	1.00	41.98	C
ATOM	1951	CG	LEU	862	17.987	28.298	10.587	1.00	49.48	C
ATOM	1952	CD1	LEU	862	18.036	29.176	9.346	1.00	46.04	C
ATOM	1953	CD2	LEU	862	18.245	26.832	10.228	1.00	47.86	C
ATOM	1954	C	LEU	862	17.272	30.273	12.642	1.00	40.85	C
ATOM	1955	O	LEU	862	16.353	30.720	11.954	1.00	45.44	O
ATOM	1956	N	LEU	863	17.108	29.839	13.900	1.00	38.85	N
ATOM	1958	CA	LEU	863	15.807	29.824	14.575	1.00	37.02	C
ATOM	1959	CB	LEU	863	15.915	29.232	15.980	1.00	43.64	C
ATOM	1960	CG	LEU	863	15.888	27.707	16.086	1.00	42.37	C
ATOM	1961	CD1	LEU	863	15.854	27.238	17.548	1.00	35.50	C
ATOM	1962	CD2	LEU	863	14.671	27.219	15.334	1.00	35.55	C
ATOM	1963	C	LEU	863	15.265	31.223	14.689	1.00	35.94	C
ATOM	1964	O	LEU	863	14.075	31.459	14.455	1.00	36.06	O
ATOM	1965	N	ASP	864	16.161	32.142	15.041	1.00	35.57	N
ATOM	1967	CA	ASP	864	15.845	33.564	15.196	1.00	37.53	C
ATOM	1968	CB	ASP	864	17.051	34.299	15.824	1.00	29.27	C
ATOM	1969	CG	ASP	864	17.214	34.005	17.334	1.00	39.10	C
ATOM	1970	OD1	ASP	864	16.388	33.270	17.927	1.00	42.54	O
ATOM	1971	OD2	ASP	864	18.174	34.526	17.947	1.00	37.49	O
ATOM	1972	C	ASP	864	15.341	34.254	13.898	1.00	38.46	C
ATOM	1973	O	ASP	864	14.455	35.123	13.959	1.00	36.51	O
ATOM	1974	N	SER	865	15.843	33.796	12.740	1.00	40.46	N
ATOM	1976	CA	SER	865	15.476	34.302	11.393	1.00	35.87	C
ATOM	1977	CB	SER	865	16.235	33.551	10.284	1.00	34.07	C
ATOM	1978	OG	SER	865	17.577	33.266	10.622	1.00	46.76	O
ATOM	1980	C	SER	865	14.004	34.116	11.058	1.00	37.22	C
ATOM	1981	O	SER	865	13.454	34.844	10.231	1.00	46.57	O
ATOM	1982	N	VAL	866	13.398	33.095	11.650	1.00	35.77	N
ATOM	1984	CA	VAL	866	12.013	32.752	11.399	1.00	35.13	C
ATOM	1985	CB	VAL	866	11.686	31.354	12.004	1.00	27.91	C
ATOM	1986	CG1	VAL	866	10.252	30.944	11.666	1.00	22.22	C
ATOM	1987	CG2	VAL	866	12.666	30.322	11.482	1.00	33.78	C
ATOM	1988	C	VAL	866	11.031	33.779	11.950	1.00	38.58	C
ATOM	1989	O	VAL	866	9.973	34.057	11.353	1.00	36.20	O

FIG. 6 CONT'D

ATOM	1990	N	GLN	867	11.395	34.366	13.081	1.00	39.58	N
ATOM	1992	CA	GLN	867	10.525	35.342	13.735	1.00	43.96	C
ATOM	1993	CB	GLN	867	11.039	35.603	15.163	1.00	47.82	C
ATOM	1994	CG	GLN	867	11.248	34.307	15.987	1.00	37.53	C
ATOM	1995	CD	GLN	867	9.951	33.535	16.271	1.00	40.95	C
ATOM	1996	OE1	GLN	867	8.841	33.972	15.943	1.00	40.47	O
ATOM	1997	NE2	GLN	867	10.097	32.375	16.883	1.00	44.07	N
ATOM	2000	C	GLN	867	10.213	36.633	12.921	1.00	38.67	C
ATOM	2001	O	GLN	867	9.030	37.022	12.789	1.00	34.00	O
ATOM	2002	N	PRO	868	11.254	37.306	12.370	1.00	32.90	N
ATOM	2003	CD	PRO	868	12.690	37.069	12.631	1.00	35.45	C
ATOM	2004	CA	PRO	868	11.071	38.522	11.569	1.00	32.84	C
ATOM	2005	CB	PRO	868	12.477	38.796	11.052	1.00	34.85	C
ATOM	2006	CG	PRO	868	13.329	38.358	12.184	1.00	35.76	C
ATOM	2007	C	PRO	868	10.156	38.173	10.407	1.00	35.58	C
ATOM	2008	O	PRO	868	9.132	38.815	10.173	1.00	34.36	O
ATOM	2009	N	ILE	869	10.494	37.075	9.740	1.00	35.25	N
ATOM	2011	CA	ILE	869	9.730	36.578	8.616	1.00	31.95	C
ATOM	2012	CB	ILE	869	10.389	35.318	8.072	1.00	34.50	C
ATOM	2013	CG2	ILE	869	9.630	34.813	6.870	1.00	25.52	C
ATOM	2014	CG1	ILE	869	11.841	35.639	7.697	1.00	31.97	C
ATOM	2015	CD1	ILE	869	12.604	34.477	7.120	1.00	36.91	C
ATOM	2016	C	ILE	869	8.284	36.304	9.002	1.00	28.05	C
ATOM	2017	O	ILE	869	7.359	36.758	8.332	1.00	33.69	O
ATOM	2018	N	ALA	870	8.089	35.599	10.109	1.00	29.58	N
ATOM	2020	CA	ALA	870	6.750	35.276	10.593	1.00	30.48	C
ATOM	2021	CB	ALA	870	6.838	34.402	11.825	1.00	27.17	C
ATOM	2022	C	ALA	870	6.010	36.567	10.913	1.00	34.81	C
ATOM	2023	O	ALA	870	4.793	36.692	10.672	1.00	31.33	O
ATOM	2024	N	ARG	871	6.754	37.534	11.441	1.00	35.08	N
ATOM	2026	CA	ARG	871	6.201	38.845	11.766	1.00	38.73	C
ATOM	2027	CB	ARG	871	7.303	39.754	12.271	1.00	42.63	C
ATOM	2028	CG	ARG	871	6.935	41.209	12.267	1.00	48.87	C
ATOM	2029	CD	ARG	871	6.488	41.628	13.610	1.00	39.03	C
ATOM	2030	NE	ARG	871	5.783	42.900	13.554	1.00	54.34	N
ATOM	2032	CZ	ARG	871	5.420	43.599	14.629	1.00	58.85	C
ATOM	2033	NH1	ARG	871	5.717	43.140	15.841	1.00	58.33	N
ATOM	2036	NH2	ARG	871	4.700	44.713	14.497	1.00	67.98	N
ATOM	2039	C	ARG	871	5.587	39.457	10.509	1.00	36.69	C
ATOM	2040	O	ARG	871	4.411	39.824	10.496	1.00	33.58	O
ATOM	2041	N	GLU	872	6.388	39.518	9.447	1.00	33.87	N
ATOM	2043	CA	GLU	872	5.954	40.047	8.149	1.00	36.69	C
ATOM	2044	CB	GLU	872	7.074	39.920	7.099	1.00	48.05	C
ATOM	2045	CG	GLU	872	7.897	41.206	6.847	1.00	57.85	C
ATOM	2046	CD	GLU	872	8.928	41.037	5.731	1.00	68.10	C
ATOM	2047	OE1	GLU	872	8.722	41.566	4.606	1.00	66.63	O
ATOM	2048	OE2	GLU	872	9.952	40.366	5.990	1.00	74.25	O
ATOM	2049	C	GLU	872	4.721	39.346	7.610	1.00	35.07	C
ATOM	2050	O	GLU	872	3.835	39.982	7.039	1.00	38.97	O
ATOM	2051	N	LEU	873	4.671	38.027	7.747	1.00	37.62	N
ATOM	2053	CA	LEU	873	3.528	37.281	7.244	1.00	35.57	C
ATOM	2054	CB	LEU	873	3.794	35.790	7.331	1.00	46.12	C
ATOM	2055	CG	LEU	873	5.003	35.377	6.498	1.00	44.82	C
ATOM	2056	CD1	LEU	873	5.185	33.921	6.706	1.00	46.86	C
ATOM	2057	CD2	LEU	873	4.807	35.680	5.024	1.00	41.83	C
ATOM	2058	C	LEU	873	2.295	37.630	8.027	1.00	36.96	C

FIG. 6 CONT'D

ATOM	2059	O	LEU	873	1.187	37.664	7.475	1.00 37.28	O
ATOM	2060	N	HIS	874	2.505	37.887	9.320	1.00 32.90	N
ATOM	2062	CA	HIS	874	1.430	38.269	10.242	1.00 37.34	C
ATOM	2063	CB	HIS	874	1.997	38.405	11.660	1.00 42.16	C
ATOM	2064	CG	HIS	874	2.251	37.099	12.352	1.00 46.12	C
ATOM	2065	CD2	HIS	874	3.339	36.643	13.015	1.00 41.95	C
ATOM	2066	ND1	HIS	874	1.296	36.104	12.440	1.00 42.36	N
ATOM	2068	CE1	HIS	874	1.790	35.088	13.130	1.00 41.59	C
ATOM	2069	NE2	HIS	874	3.028	35.390	13.486	1.00 44.61	N
ATOM	2071	C	HIS	874	0.775	39.603	9.828	1.00 38.25	C
ATOM	2072	O	HIS	874	-0.457	39.758	9.814	1.00 36.81	O
ATOM	2073	N	GLN	875	1.628	40.572	9.520	1.00 38.39	N
ATOM	2075	CA	GLN	875	1.217	41.906	9.090	1.00 36.36	C
ATOM	2076	CB	GLN	875	2.471	42.727	8.765	1.00 38.26	C
ATOM	2077	CG	GLN	875	2.247	44.182	8.555	1.00 44.03	C
ATOM	2078	CD	GLN	875	1.775	44.875	9.800	1.00 47.03	C
ATOM	2079	OE1	GLN	875	2.554	45.079	10.754	1.00 42.92	O
ATOM	2080	NE2	GLN	875	0.504	45.272	9.799	1.00 34.68	N
ATOM	2083	C	GLN	875	0.363	41.731	7.845	1.00 34.57	C
ATOM	2084	O	GLN	875	-0.822	42.017	7.846	1.00 42.38	O
ATOM	2085	N	PHE	876	0.943	41.081	6.849	1.00 33.26	N
ATOM	2087	CA	PHE	876	0.284	40.845	5.582	1.00 33.07	C
ATOM	2088	CB	PHE	876	1.212	40.017	4.692	1.00 39.86	C
ATOM	2089	CG	PHE	876	0.676	39.782	3.313	1.00 39.61	C
ATOM	2090	CD1	PHE	876	1.163	40.507	2.248	1.00 39.57	C
ATOM	2091	CD2	PHE	876	-0.320	38.846	3.085	1.00 41.67	C
ATOM	2092	CE1	PHE	876	0.665	40.318	0.991	1.00 40.20	C
ATOM	2093	CE2	PHE	876	-0.823	38.650	1.838	1.00 44.63	C
ATOM	2094	CZ	PHE	876	-0.329	39.385	0.780	1.00 49.53	C
ATOM	2095	C	PHE	876	-1.070	40.161	5.677	1.00 35.06	C
ATOM	2096	O	PHE	876	-2.036	40.573	5.032	1.00 34.48	O
ATOM	2097	N	THR	877	-1.126	39.053	6.405	1.00 40.28	N
ATOM	2099	CA	THR	877	-2.380	38.320	6.505	1.00 38.84	C
ATOM	2100	CB	THR	877	-2.193	36.900	7.135	1.00 33.79	C
ATOM	2101	OG1	THR	877	-3.364	36.117	6.886	1.00 38.07	O
ATOM	2103	CG2	THR	877	-1.937	36.956	8.640	1.00 26.06	C
ATOM	2104	C	THR	877	-3.450	39.157	7.208	1.00 41.69	C
ATOM	2105	O	THR	877	-4.594	39.193	6.767	1.00 41.63	O
ATOM	2106	N	PHE	878	-3.062	39.889	8.251	1.00 39.96	N
ATOM	2108	CA	PHE	878	-3.997	40.737	8.984	1.00 38.02	C
ATOM	2109	CB	PHE	878	-3.248	41.450	10.109	1.00 41.25	C
ATOM	2110	CG	PHE	878	-4.035	42.540	10.764	1.00 45.72	C
ATOM	2111	CD1	PHE	878	-5.318	42.298	11.237	1.00 47.19	C
ATOM	2112	CD2	PHE	878	-3.490	43.810	10.910	1.00 47.82	C
ATOM	2113	CE1	PHE	878	-6.045	43.296	11.842	1.00 52.43	C
ATOM	2114	CE2	PHE	878	-4.208	44.813	11.515	1.00 44.62	C
ATOM	2115	CZ	PHE	878	-5.488	44.563	11.983	1.00 50.04	C
ATOM	2116	C	PHE	878	-4.600	41.760	8.006	1.00 38.85	C
ATOM	2117	O	PHE	878	-5.821	41.922	7.916	1.00 33.84	O
ATOM	2118	N	ASP	879	-3.717	42.398	7.243	1.00 41.64	N
ATOM	2120	CA	ASP	879	-4.078	43.395	6.242	1.00 44.39	C
ATOM	2121	CB	ASP	879	-2.799	43.987	5.597	1.00 50.23	C
ATOM	2122	CG	ASP	879	-1.938	44.849	6.595	1.00 65.18	C
ATOM	2123	OD1	ASP	879	-2.253	44.919	7.821	1.00 64.91	O
ATOM	2124	OD2	ASP	879	-0.930	45.461	6.140	1.00 57.87	O
ATOM	2125	C	ASP	879	-4.975	42.733	5.201	1.00 41.74	C

FIG. 6 CONT'D

ATOM	2126	O	ASP	879	-6.013	43.272	4.797	1.00	45.58	O
ATOM	2127	N	LEU	880	-4.581	41.542	4.784	1.00	39.59	N
ATOM	2129	CA	LEU	880	-5.349	40.778	3.824	1.00	41.16	C
ATOM	2130	CB	LEU	880	-4.594	39.483	3.484	1.00	41.26	C
ATOM	2131	CG	LEU	880	-5.117	38.492	2.429	1.00	46.22	C
ATOM	2132	CD1	LEU	880	-5.910	39.174	1.299	1.00	39.53	C
ATOM	2133	CD2	LEU	880	-3.925	37.702	1.873	1.00	45.58	C
ATOM	2134	C	LEU	880	-6.737	40.477	4.404	1.00	41.39	C
ATOM	2135	O	LEU	880	-7.720	40.472	3.682	1.00	46.61	O
ATOM	2136	N	LEU	881	-6.826	40.273	5.713	1.00	46.94	N
ATOM	2138	CA	LEU	881	-8.113	39.974	6.330	1.00	46.60	C
ATOM	2139	CB	LEU	881	-7.964	39.468	7.775	1.00	38.43	C
ATOM	2140	CG	LEU	881	-9.282	39.274	8.551	1.00	37.70	C
ATOM	2141	CD1	LEU	881	-10.162	38.204	7.887	1.00	30.98	C
ATOM	2142	CD2	LEU	881	-8.979	38.918	9.997	1.00	30.24	C
ATOM	2143	C	LEU	881	-9.028	41.185	6.310	1.00	50.61	C
ATOM	2144	O	LEU	881	-10.188	41.070	5.925	1.00	50.82	O
ATOM	2145	N	ILE	882	-8.531	42.341	6.746	1.00	48.70	N
ATOM	2147	CA	ILE	882	-9.390	43.517	6.752	1.00	55.61	C
ATOM	2148	CB	ILE	882	-8.797	44.720	7.603	1.00	54.73	C
ATOM	2149	CG2	ILE	882	-8.566	44.271	9.054	1.00	42.17	C
ATOM	2150	CG1	ILE	882	-7.489	45.252	7.008	1.00	58.00	C
ATOM	2151	CD1	ILE	882	-6.825	46.382	7.811	1.00	61.98	C
ATOM	2152	C	ILE	882	-9.806	43.885	5.314	1.00	53.19	C
ATOM	2153	O	ILE	882	-10.966	44.227	5.076	1.00	56.55	O
ATOM	2154	N	LYS	883	-8.917	43.674	4.343	1.00	51.98	N
ATOM	2156	CA	LYS	883	-9.229	43.976	2.939	1.00	53.80	C
ATOM	2157	CB	LYS	883	-7.976	44.008	2.073	1.00	49.48	C
ATOM	2158	CG	LYS	883	-7.056	45.152	2.279	1.00	51.98	C
ATOM	2159	CD	LYS	883	-5.970	45.061	1.236	1.00	57.39	C
ATOM	2160	CE	LYS	883	-4.752	45.885	1.601	1.00	65.28	C
ATOM	2161	NZ	LYS	883	-3.755	45.773	0.507	1.00	72.32	N
ATOM	2165	C	LYS	883	-10.126	42.935	2.296	1.00	56.69	C
ATOM	2166	O	LYS	883	-10.888	43.257	1.389	1.00	56.03	O
ATOM	2167	N	SER	884	-10.000	41.687	2.758	1.00	64.45	N
ATOM	2169	CA	SER	884	-10.721	40.515	2.228	1.00	60.51	C
ATOM	2170	CB	SER	884	-10.873	39.434	3.304	1.00	60.86	C
ATOM	2171	OG	SER	884	-11.559	39.933	4.437	1.00	69.00	O
ATOM	2173	C	SER	884	-12.055	40.765	1.543	1.00	57.37	C
ATOM	2174	O	SER	884	-12.167	40.549	0.334	1.00	55.96	O
ATOM	2175	N	HIS	885	-13.029	41.258	2.308	1.00	59.05	N
ATOM	2177	CA	HIS	885	-14.376	41.558	1.826	1.00	68.14	C
ATOM	2178	CB	HIS	885	-15.091	42.532	2.781	1.00	74.25	C
ATOM	2179	CG	HIS	885	-14.848	42.258	4.241	1.00	79.02	C
ATOM	2180	CD2	HIS	885	-15.545	41.521	5.135	1.00	74.74	C
ATOM	2181	ND1	HIS	885	-13.766	42.770	4.919	1.00	75.36	N
ATOM	2183	CE1	HIS	885	-13.802	42.360	6.178	1.00	69.84	C
ATOM	2184	NE2	HIS	885	-14.871	41.599	6.335	1.00	76.42	N
ATOM	2186	C	HIS	885	-14.388	42.167	0.424	1.00	74.11	C
ATOM	2187	O	HIS	885	-14.901	41.561	-0.515	1.00	78.87	O
ATOM	2188	N	MET	886	-13.813	43.358	0.284	1.00	77.20	N
ATOM	2190	CA	MET	886	-13.780	44.065	-1.003	1.00	75.99	C
ATOM	2191	CB	MET	886	-13.570	45.582	-0.755	1.00	87.39	C
ATOM	2192	CG	MET	886	-12.135	46.127	-0.979	1.00	94.48	C
ATOM	2193	SD	MET	886	-11.788	47.728	-0.157	1.00	94.87	S
ATOM	2194	CE	MET	886	-10.212	48.246	-1.001	1.00	94.14	C

FIG. 6 CONT'D

ATOM	2195	C	MET	886	-12.804	43.540	-2.083	1.00 66.55	C
ATOM	2196	O	MET	886	-12.844	44.000	-3.225	1.00 63.97	O
ATOM	2197	N	VAL	887	-11.942	42.584	-1.738	1.00 60.32	N
ATOM	2199	CA	VAL	887	-10.968	42.057	-2.702	1.00 54.75	C
ATOM	2200	CB	VAL	887	-9.525	42.334	-2.213	1.00 48.73	C
ATOM	2201	CG1	VAL	887	-9.081	41.277	-1.221	1.00 55.82	C
ATOM	2202	CG2	VAL	887	-8.578	42.459	-3.377	1.00 42.79	C
ATOM	2203	C	VAL	887	-11.146	40.564	-3.026	1.00 56.80	C
ATOM	2204	O	VAL	887	-10.263	39.931	-3.624	1.00 52.84	O
ATOM	2205	N	SER	888	-12.293	40.033	-2.599	1.00 60.63	N
ATOM	2207	CA	SER	888	-12.752	38.643	-2.786	1.00 60.83	C
ATOM	2208	CB	SER	888	-13.368	38.463	-4.169	1.00 51.52	C
ATOM	2209	OG	SER	888	-12.417	38.680	-5.181	1.00 58.27	O
ATOM	2211	C	SER	888	-11.912	37.401	-2.406	1.00 65.27	C
ATOM	2212	O	SER	888	-12.196	36.292	-2.885	1.00 62.05	O
ATOM	2213	N	VAL	889	-10.918	37.579	-1.529	1.00 70.51	N
ATOM	2215	CA	VAL	889	-10.079	36.475	-1.036	1.00 69.77	C
ATOM	2216	CB	VAL	889	-8.740	37.003	-0.461	1.00 68.58	C
ATOM	2217	CG1	VAL	889	-7.880	35.843	-0.016	1.00 73.27	C
ATOM	2218	CG2	VAL	889	-8.006	37.859	-1.489	1.00 65.97	C
ATOM	2219	C	VAL	889	-10.894	35.856	0.115	1.00 71.90	C
ATOM	2220	O	VAL	889	-11.475	36.609	0.910	1.00 70.16	O
ATOM	2221	N	ASP	890	-10.969	34.520	0.203	1.00 74.76	N
ATOM	2223	CA	ASP	890	-11.758	33.870	1.271	1.00 72.71	C
ATOM	2224	CB	ASP	890	-12.783	32.857	0.666	1.00 72.91	C
ATOM	2225	CG	ASP	890	-12.332	31.385	0.735	1.00 80.84	C
ATOM	2226	OD1	ASP	890	-13.045	30.618	1.413	1.00 78.59	O
ATOM	2227	OD2	ASP	890	-11.326	30.981	0.093	1.00 76.21	O
ATOM	2228	C	ASP	890	-10.920	33.314	2.457	1.00 69.55	C
ATOM	2229	O	ASP	890	-9.783	32.831	2.270	1.00 70.86	O
ATOM	2230	N	PHE	891	-11.431	33.508	3.680	1.00 59.70	N
ATOM	2232	CA	PHE	891	-10.746	33.068	4.902	1.00 52.91	C
ATOM	2233	CB	PHE	891	-10.474	34.274	5.848	1.00 55.80	C
ATOM	2234	CG	PHE	891	-9.223	35.088	5.518	1.00 47.41	C
ATOM	2235	CD1	PHE	891	-9.250	36.101	4.554	1.00 40.14	C
ATOM	2236	CD2	PHE	891	-8.027	34.837	6.171	1.00 45.78	C
ATOM	2237	CE1	PHE	891	-8.107	36.842	4.246	1.00 34.67	C
ATOM	2238	CE2	PHE	891	-6.876	35.585	5.862	1.00 46.05	C
ATOM	2239	CZ	PHE	891	-6.922	36.582	4.900	1.00 37.02	C
ATOM	2240	C	PHE	891	-11.598	32.045	5.665	1.00 49.30	C
ATOM	2241	O	PHE	891	-12.740	32.326	6.012	1.00 50.65	O
ATOM	2242	N	PRO	892	-11.052	30.845	5.926	1.00 44.99	N
ATOM	2243	CD	PRO	892	-9.737	30.353	5.480	1.00 46.20	C
ATOM	2244	CA	PRO	892	-11.782	29.806	6.660	1.00 39.76	C
ATOM	2245	CB	PRO	892	-10.792	28.648	6.669	1.00 45.27	C
ATOM	2246	CG	PRO	892	-9.970	28.878	5.420	1.00 46.05	C
ATOM	2247	C	PRO	892	-11.976	30.370	8.058	1.00 44.96	C
ATOM	2248	O	PRO	892	-11.052	30.952	8.621	1.00 46.87	O
ATOM	2249	N	GLU	893	-13.176	30.234	8.604	1.00 51.64	N
ATOM	2251	CA	GLU	893	-13.508	30.792	9.914	1.00 51.25	C
ATOM	2252	CB	GLU	893	-14.937	30.437	10.304	1.00 59.05	C
ATOM	2253	CG	GLU	893	-15.987	31.401	9.724	1.00 75.65	C
ATOM	2254	CD	GLU	893	-15.800	31.699	8.224	1.00 82.95	C
ATOM	2255	OE1	GLU	893	-15.762	32.891	7.845	1.00 86.37	O
ATOM	2256	OE2	GLU	893	-15.706	30.745	7.418	1.00 84.06	O
ATOM	2257	C	GLU	893	-12.577	30.549	11.077	1.00 52.74	C

FIG. 6 CONT'D

ATOM	2258	O	GLU	893	-12.321	31.462	11.858	1.00	58.39	O
ATOM	2259	N	MET	894	-12.043	29.348	11.205	1.00	52.94	N
ATOM	2261	CA	MET	894	-11.152	29.075	12.329	1.00	57.23	C
ATOM	2262	CB	MET	894	-10.720	27.607	12.332	1.00	59.88	C
ATOM	2263	CG	MET	894	-9.861	27.205	13.522	1.00	68.32	C
ATOM	2264	SD	MET	894	-9.861	25.428	13.821	1.00	73.67	S
ATOM	2265	CE	MET	894	-9.322	24.840	12.166	1.00	72.54	C
ATOM	2266	C	MET	894	-9.942	29.975	12.239	1.00	57.71	C
ATOM	2267	O	MET	894	-9.458	30.518	13.230	1.00	60.99	O
ATOM	2268	N	MET	895	-9.466	30.130	11.021	1.00	61.08	N
ATOM	2270	CA	MET	895	-8.311	30.948	10.744	1.00	58.05	C
ATOM	2271	CB	MET	895	-7.751	30.527	9.396	1.00	57.93	C
ATOM	2272	CG	MET	895	-6.936	31.548	8.720	1.00	67.27	C
ATOM	2273	SD	MET	895	-6.668	30.991	7.072	1.00	79.81	S
ATOM	2274	CE	MET	895	-4.870	31.161	6.982	1.00	78.99	C
ATOM	2275	C	MET	895	-8.679	32.431	10.789	1.00	56.79	C
ATOM	2276	O	MET	895	-7.979	33.226	11.422	1.00	56.34	O
ATOM	2277	N	ALA	896	-9.786	32.802	10.152	1.00	49.66	N
ATOM	2279	CA	ALA	896	-10.219	34.186	10.170	1.00	46.91	C
ATOM	2280	CB	ALA	896	-11.616	34.311	9.591	1.00	45.04	C
ATOM	2281	C	ALA	896	-10.211	34.621	11.627	1.00	50.19	C
ATOM	2282	O	ALA	896	-9.655	35.672	11.971	1.00	55.53	O
ATOM	2283	N	GLU	897	-10.737	33.759	12.496	1.00	52.29	N
ATOM	2285	CA	GLU	897	-10.805	34.053	13.928	1.00	52.77	C
ATOM	2286	CB	GLU	897	-11.612	32.990	14.664	1.00	54.94	C
ATOM	2287	CG	GLU	897	-11.927	33.355	16.111	1.00	65.44	C
ATOM	2288	CD	GLU	897	-13.217	32.725	16.600	1.00	75.27	C
ATOM	2289	OE1	GLU	897	-14.284	33.102	16.074	1.00	78.93	O
ATOM	2290	OE2	GLU	897	-13.167	31.868	17.511	1.00	79.28	O
ATOM	2291	C	GLU	897	-9.442	34.244	14.591	1.00	48.32	C
ATOM	2292	O	GLU	897	-9.253	35.144	15.402	1.00	49.52	O
ATOM	2293	N	ILE	898	-8.477	33.417	14.241	1.00	45.91	N
ATOM	2295	CA	ILE	898	-7.160	33.561	14.836	1.00	43.63	C
ATOM	2296	CB	ILE	898	-6.275	32.288	14.567	1.00	45.82	C
ATOM	2297	CG2	ILE	898	-4.776	32.537	14.847	1.00	34.18	C
ATOM	2298	CG1	ILE	898	-6.797	31.125	15.430	1.00	48.14	C
ATOM	2299	CD1	ILE	898	-5.911	29.894	15.425	1.00	60.11	C
ATOM	2300	C	ILE	898	-6.510	34.843	14.323	1.00	41.42	C
ATOM	2301	O	ILE	898	-5.891	35.578	15.087	1.00	41.91	O
ATOM	2302	N	ILE	899	-6.734	35.177	13.064	1.00	37.89	N
ATOM	2304	CA	ILE	899	-6.105	36.372	12.526	1.00	40.46	C
ATOM	2305	CB	ILE	899	-6.290	36.486	10.986	1.00	46.34	C
ATOM	2306	CG2	ILE	899	-5.612	37.759	10.448	1.00	45.77	C
ATOM	2307	CG1	ILE	899	-5.722	35.250	10.280	1.00	51.08	C
ATOM	2308	CD1	ILE	899	-4.239	34.978	10.550	1.00	53.92	C
ATOM	2309	C	ILE	899	-6.640	37.624	13.202	1.00	39.91	C
ATOM	2310	O	ILE	899	-5.880	38.533	13.524	1.00	36.62	O
ATOM	2311	N	SER	900	-7.927	37.612	13.520	1.00	39.54	N
ATOM	2313	CA	SER	900	-8.576	38.764	14.129	1.00	39.63	C
ATOM	2314	CB	SER	900	-10.048	38.823	13.670	1.00	37.01	C
ATOM	2315	OG	SER	900	-10.963	38.377	14.652	1.00	40.29	O
ATOM	2317	C	SER	900	-8.474	38.925	15.652	1.00	41.36	C
ATOM	2318	O	SER	900	-8.821	39.970	16.188	1.00	46.90	O
ATOM	2319	N	VAL	901	-7.942	37.938	16.350	1.00	34.58	N
ATOM	2321	CA	VAL	901	-7.889	38.027	17.799	1.00	32.25	C
ATOM	2322	CB	VAL	901	-8.844	36.967	18.443	1.00	40.69	C

FIG. 6 CONT'D

ATOM	2323	CG1	VAL	901	-8.793	37.045	19.976	1.00	37.09	C
ATOM	2324	CG2	VAL	901	-10.273	37.146	17.930	1.00	37.39	C
ATOM	2325	C	VAL	901	-6.516	37.812	18.388	1.00	33.93	C
ATOM	2326	O	VAL	901	-6.116	38.496	19.325	1.00	37.49	O
ATOM	2327	N	GLN	902	-5.813	36.820	17.865	1.00	38.32	N
ATOM	2329	CA	GLN	902	-4.504	36.475	18.376	1.00	36.30	C
ATOM	2330	CB	GLN	902	-4.247	34.958	18.276	1.00	36.78	C
ATOM	2331	CG	GLN	902	-5.309	34.053	18.926	1.00	41.09	C
ATOM	2332	CD	GLN	902	-5.529	34.320	20.418	1.00	47.88	C
ATOM	2333	OE1	GLN	902	-6.664	34.277	20.899	1.00	56.15	O
ATOM	2334	NE2	GLN	902	-4.447	34.587	21.155	1.00	43.52	N
ATOM	2337	C	GLN	902	-3.432	37.222	17.639	1.00	39.26	C
ATOM	2338	O	GLN	902	-2.419	37.566	18.234	1.00	41.22	O
ATOM	2339	N	VAL	903	-3.621	37.449	16.340	1.00	40.86	N
ATOM	2341	CA	VAL	903	-2.611	38.167	15.569	1.00	38.57	C
ATOM	2342	CB	VAL	903	-2.841	38.035	14.028	1.00	42.29	C
ATOM	2343	CG1	VAL	903	-1.947	38.994	13.270	1.00	39.28	C
ATOM	2344	CG2	VAL	903	-2.503	36.622	13.574	1.00	39.72	C
ATOM	2345	C	VAL	903	-2.431	39.624	16.026	1.00	37.36	C
ATOM	2346	O	VAL	903	-1.294	40.077	16.171	1.00	39.48	O
ATOM	2347	N	PRO	904	-3.534	40.366	16.292	1.00	30.75	N
ATOM	2348	CD	PRO	904	-4.962	40.088	16.042	1.00	34.37	C
ATOM	2349	CA	PRO	904	-3.373	41.753	16.738	1.00	32.91	C
ATOM	2350	CB	PRO	904	-4.797	42.161	17.092	1.00	29.43	C
ATOM	2351	CG	PRO	904	-5.571	41.493	16.035	1.00	30.40	C
ATOM	2352	C	PRO	904	-2.436	41.878	17.945	1.00	36.72	C
ATOM	2353	O	PRO	904	-1.624	42.801	18.019	1.00	40.29	O
ATOM	2354	N	LYS	905	-2.489	40.909	18.851	1.00	36.01	N
ATOM	2356	CA	LYS	905	-1.632	40.937	20.031	1.00	32.07	C
ATOM	2357	CB	LYS	905	-1.995	39.807	21.022	1.00	34.01	C
ATOM	2358	CG	LYS	905	-3.485	39.698	21.377	1.00	37.81	C
ATOM	2359	CD	LYS	905	-3.751	38.653	22.476	1.00	51.29	C
ATOM	2360	CE	LYS	905	-5.233	38.624	22.886	1.00	51.15	C
ATOM	2361	NZ	LYS	905	-5.552	37.658	23.987	1.00	63.78	N
ATOM	2365	C	LYS	905	-0.149	40.868	19.677	1.00	30.44	C
ATOM	2366	O	LYS	905	0.688	41.365	20.422	1.00	33.55	O
ATOM	2367	N	ILE	906	0.185	40.258	18.545	1.00	38.99	N
ATOM	2369	CA	ILE	906	1.588	40.103	18.142	1.00	43.43	C
ATOM	2370	CB	ILE	906	1.818	38.828	17.217	1.00	41.03	C
ATOM	2371	CG2	ILE	906	3.289	38.764	16.745	1.00	35.00	C
ATOM	2372	CG1	ILE	906	1.453	37.545	17.993	1.00	41.68	C
ATOM	2373	CD1	ILE	906	1.386	36.270	17.189	1.00	36.91	C
ATOM	2374	C	ILE	906	2.076	41.353	17.449	1.00	46.59	C
ATOM	2375	O	ILE	906	3.203	41.817	17.688	1.00	46.25	O
ATOM	2376	N	LEU	907	1.217	41.891	16.587	1.00	50.54	N
ATOM	2378	CA	LEU	907	1.516	43.111	15.831	1.00	47.53	C
ATOM	2379	CB	LEU	907	0.437	43.324	14.751	1.00	43.43	C
ATOM	2380	CG	LEU	907	0.323	42.131	13.782	1.00	31.27	C
ATOM	2381	CD1	LEU	907	-0.857	42.290	12.901	1.00	29.15	C
ATOM	2382	CD2	LEU	907	1.580	41.967	12.953	1.00	29.66	C
ATOM	2383	C	LEU	907	1.639	44.317	16.784	1.00	42.06	C
ATOM	2384	O	LEU	907	2.496	45.199	16.590	1.00	41.92	O
ATOM	2385	N	SER	908	0.851	44.282	17.858	1.00	36.02	N
ATOM	2387	CA	SER	908	0.871	45.328	18.852	1.00	41.77	C
ATOM	2388	CB	SER	908	-0.519	45.531	19.479	1.00	44.15	C
ATOM	2389	OG	SER	908	-0.913	44.474	20.334	1.00	47.22	O

FIG. 6 CONT'D

ATOM	2391	C	SER	908	1.943	45.131	19.931	1.00	45.83	C
ATOM	2392	O	SER	908	2.115	45.985	20.788	1.00	57.61	O
ATOM	2393	N	GLY	909	2.684	44.030	19.886	1.00	40.63	N
ATOM	2395	CA	GLY	909	3.726	43.813	20.877	1.00	31.68	C
ATOM	2396	C	GLY	909	3.324	43.227	22.233	1.00	37.71	C
ATOM	2397	O	GLY	909	4.173	43.163	23.129	1.00	42.65	O
ATOM	2398	N	LYS	910	2.071	42.791	22.401	1.00	33.50	N
ATOM	2400	CA	LYS	910	1.619	42.182	23.673	1.00	42.03	C
ATOM	2401	CB	LYS	910	0.100	42.320	23.805	1.00	41.10	C
ATOM	2402	CG	LYS	910	-0.357	43.751	23.582	1.00	45.52	C
ATOM	2403	CD	LYS	910	-1.830	43.904	23.726	1.00	40.97	C
ATOM	2404	CE	LYS	910	-2.190	43.976	25.163	1.00	42.32	C
ATOM	2405	NZ	LYS	910	-3.651	43.819	25.260	1.00	53.43	N
ATOM	2409	C	LYS	910	2.064	40.702	23.839	1.00	41.10	C
ATOM	2410	O	LYS	910	2.036	40.137	24.932	1.00	39.99	O
ATOM	2411	N	VAL	911	2.497	40.114	22.728	1.00	42.05	N
ATOM	2413	CA	VAL	911	2.992	38.746	22.624	1.00	35.21	C
ATOM	2414	CB	VAL	911	2.025	37.872	21.822	1.00	29.65	C
ATOM	2415	CG1	VAL	911	2.661	36.551	21.476	1.00	33.30	C
ATOM	2416	CG2	VAL	911	0.736	37.674	22.588	1.00	35.10	C
ATOM	2417	C	VAL	911	4.267	38.912	21.806	1.00	36.16	C
ATOM	2418	O	VAL	911	4.224	39.387	20.671	1.00	37.87	O
ATOM	2419	N	LYS	912	5.396	38.504	22.358	1.00	35.80	N
ATOM	2421	CA	LYS	912	6.638	38.677	21.653	1.00	36.47	C
ATOM	2422	CB	LYS	912	7.483	39.752	22.347	1.00	37.13	C
ATOM	2423	CG	LYS	912	7.952	39.353	23.729	0.00	38.33	C
ATOM	2424	CD	LYS	912	8.846	40.405	24.332	0.00	39.07	C
ATOM	2425	CE	LYS	912	9.124	40.089	25.784	0.00	39.77	C
ATOM	2426	NZ	LYS	912	9.862	41.200	26.423	0.00	40.28	N
ATOM	2430	C	LYS	912	7.451	37.409	21.556	1.00	40.23	C
ATOM	2431	O	LYS	912	7.293	36.472	22.334	1.00	39.68	O
ATOM	2432	N	PRO	913	8.266	37.333	20.517	1.00	39.61	N
ATOM	2433	CD	PRO	913	8.060	38.134	19.296	1.00	42.22	C
ATOM	2434	CA	PRO	913	9.146	36.208	20.249	1.00	40.14	C
ATOM	2435	CB	PRO	913	9.711	36.564	18.875	1.00	41.93	C
ATOM	2436	CG	PRO	913	8.534	37.200	18.210	1.00	44.72	C
ATOM	2437	C	PRO	913	10.247	36.181	21.301	1.00	36.50	C
ATOM	2438	O	PRO	913	10.565	37.200	21.893	1.00	38.67	O
ATOM	2439	N	ILE	914	10.813	35.008	21.538	1.00	34.68	N
ATOM	2441	CA	ILE	914	11.883	34.848	22.497	1.00	36.82	C
ATOM	2442	CB	ILE	914	11.625	33.663	23.434	1.00	38.93	C
ATOM	2443	CG2	ILE	914	12.743	33.540	24.435	1.00	46.36	C
ATOM	2444	CG1	ILE	914	10.311	33.834	24.173	1.00	32.49	C
ATOM	2445	CD1	ILE	914	9.917	32.567	24.899	1.00	39.70	C
ATOM	2446	C	ILE	914	13.085	34.508	21.654	1.00	40.11	C
ATOM	2447	O	ILE	914	13.129	33.460	21.029	1.00	43.44	O
ATOM	2448	N	TYR	915	14.047	35.409	21.603	1.00	45.62	N
ATOM	2450	CA	TYR	915	15.235	35.191	20.798	1.00	45.53	C
ATOM	2451	CB	TYR	915	15.717	36.510	20.165	1.00	38.58	C
ATOM	2452	CG	TYR	915	14.778	37.052	19.122	1.00	36.78	C
ATOM	2453	CD1	TYR	915	13.600	37.695	19.484	1.00	38.75	C
ATOM	2454	CE1	TYR	915	12.696	38.141	18.527	1.00	49.22	C
ATOM	2455	CD2	TYR	915	15.042	36.875	17.767	1.00	47.40	C
ATOM	2456	CE2	TYR	915	14.142	37.317	16.786	1.00	52.13	C
ATOM	2457	CZ	TYR	915	12.969	37.952	17.175	1.00	56.55	C
ATOM	2458	OH	TYR	915	12.067	38.377	16.212	1.00	55.66	O

FIG. 6 CONT'D

ATOM	2460	C	TYR	915	16.352	34.582	21.608	1.00	47.03	C
ATOM	2461	O	TYR	915	16.359	34.665	22.833	1.00	51.25	O
ATOM	2462	N	PHE	916	17.298	33.964	20.915	1.00	46.26	N
ATOM	2464	CA	PHE	916	18.439	33.376	21.580	1.00	44.65	C
ATOM	2465	CB	PHE	916	18.993	32.180	20.787	1.00	42.46	C
ATOM	2466	CG	PHE	916	18.213	30.915	20.991	1.00	44.06	C
ATOM	2467	CD1	PHE	916	18.670	29.948	21.875	1.00	47.18	C
ATOM	2468	CD2	PHE	916	17.006	30.705	20.326	1.00	46.38	C
ATOM	2469	CE1	PHE	916	17.939	28.789	22.098	1.00	46.95	C
ATOM	2470	CE2	PHE	916	16.263	29.553	20.540	1.00	45.51	C
ATOM	2471	CZ	PHE	916	16.732	28.594	21.426	1.00	45.10	C
ATOM	2472	C	PHE	916	19.487	34.457	21.707	1.00	44.05	C
ATOM	2473	O	PHE	916	20.132	34.568	22.738	1.00	47.61	O
ATOM	2474	N	HIS	917	19.603	35.303	20.689	1.00	46.97	N
ATOM	2476	CA	HIS	917	20.611	36.352	20.694	1.00	47.06	C
ATOM	2477	CB	HIS	917	21.524	36.170	19.471	1.00	49.03	C
ATOM	2478	CG	HIS	917	21.994	34.756	19.246	1.00	43.80	C
ATOM	2479	CD2	HIS	917	21.343	33.670	18.762	1.00	48.20	C
ATOM	2480	ND1	HIS	917	23.287	34.340	19.494	1.00	47.63	N
ATOM	2482	CE1	HIS	917	23.414	33.065	19.173	1.00	51.22	C
ATOM	2483	NE2	HIS	917	22.248	32.631	18.726	1.00	47.78	N
ATOM	2485	C	HIS	917	20.043	37.777	20.743	1.00	52.16	C
ATOM	2486	O	HIS	917	20.353	38.603	19.896	1.00	57.53	O
ATOM	2487	N	THR	918	19.206	38.052	21.735	1.00	62.03	N
ATOM	2489	CA	THR	918	18.597	39.381	21.917	1.00	72.18	C
ATOM	2490	CB	THR	918	17.378	39.309	22.847	1.00	73.07	C
ATOM	2491	OG1	THR	918	16.840	37.980	22.842	1.00	72.53	N
ATOM	2493	CG2	THR	918	16.301	40.339	22.419	1.00	76.16	C
ATOM	2494	C	THR	918	19.558	40.395	22.571	1.00	75.33	C
ATOM	2495	OT1	THR	918	19.150	41.565	22.781	1.00	78.71	N
ATOM	2496	OT2	THR	918	20.674	39.997	22.964	1.00	76.97	N
ATOM	2497	C1	R18	1000	0.414	28.070	4.103	1.00	47.66	C
ATOM	2498	C2	R18	1000	1.195	26.999	4.832	1.00	49.34	C
ATOM	2499	C3	R18	1000	2.661	27.140	4.532	1.00	53.90	C
ATOM	2500	C4	R18	1000	3.174	28.457	4.794	1.00	55.05	C
ATOM	2501	C5	R18	1000	2.367	29.553	4.780	1.00	50.29	C
ATOM	2502	C6	R18	1000	2.973	30.906	5.116	1.00	47.48	C
ATOM	2503	C7	R18	1000	2.207	32.030	4.457	1.00	46.11	C
ATOM	2504	C8	R18	1000	0.733	31.962	4.898	1.00	45.61	C
ATOM	2505	C9	R18	1000	0.124	30.597	4.514	1.00	49.94	C
ATOM	2506	C10	R18	1000	0.912	29.480	4.476	1.00	49.84	C
ATOM	2507	C11	R18	1000	-1.316	30.583	4.251	1.00	47.61	C
ATOM	2508	C12	R18	1000	-2.102	31.675	4.310	1.00	47.26	C
ATOM	2509	C13	R18	1000	-1.535	33.039	4.664	1.00	44.26	C
ATOM	2510	C14	R18	1000	-0.056	33.066	4.261	1.00	42.93	C
ATOM	2511	C15	R18	1000	0.387	34.509	4.572	1.00	43.22	C
ATOM	2512	C16	R18	1000	-0.899	35.299	4.311	1.00	41.50	C
ATOM	2513	C17	R18	1000	-2.001	34.282	3.900	1.00	43.39	C
ATOM	2514	C18	R18	1000	-1.725	33.228	6.189	1.00	41.74	C
ATOM	2515	C27	R18	1000	-2.034	34.050	2.412	1.00	40.38	C
ATOM	2516	O83	R18	1000	3.375	26.212	4.162	1.00	59.41	O
ATOM	2517	O97	R18	1000	-3.257	34.797	4.345	1.00	48.46	O
ATOM	2519	OW	WAT	1001	7.977	16.353	14.548	1.00	29.86	O
ATOM	2522	OW	WAT	1002	12.529	31.030	16.979	1.00	35.29	O
ATOM	2525	OW	WAT	1003	4.151	24.024	6.333	1.00	32.89	O
ATOM	2528	OW	WAT	1004	1.368	26.376	31.674	1.00	49.63	O

FIG. 6 CONT'D

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ATOM   2531  OW  WAT  1005       2.693  46.635  13.278  1.00 46.55      O
ATOM   2534  OW  WAT  1006      16.821  36.244  25.158  1.00 58.36      O
ATOM   2537  OW  WAT  1007       6.659  32.126  15.319  1.00 44.19      O
ATOM   2540  OW  WAT  1008       4.179  32.582  14.418  1.00 31.77      O
ATOM   2543  OW  WAT  1009      -1.370  30.527 -15.016  1.00 41.87      O
ATOM   2546  OW  WAT  1010      28.211  24.615   5.938  1.00 56.69      O
ATOM   2549  OW  WAT  1011      -7.536  14.518  23.118  1.00 42.77      O
ATOM   2552  OW  WAT  1012       7.032  36.581  14.890  1.00 40.54      O
ATOM   2555  OW  WAT  1013      18.090  34.834   6.262  1.00 66.21      O
ATOM   2558  OW  WAT  1014       5.741  29.774  22.458  1.00 37.52      O
ATOM   2561  OW  WAT  1015      29.879   8.063  10.984  1.00 53.83      O
ATOM   2564  OW  WAT  1016      17.517  11.963  20.575  1.00 51.58      O
ATOM   2567  OW  WAT  1017       7.674  37.499  32.487  1.00 46.92      O
ATOM   2570  OW  WAT  1018      -4.737  36.972 -13.426  1.00 75.71      O
ATOM   2573  OW  WAT  1019       1.207  32.439  14.426  1.00 45.58      O
ATOM   2576  OW  WAT  1020      -5.348  34.883  24.137  1.00 62.76      O
ATOM   2579  OW  WAT  1021      10.790  29.074   3.632  1.00 61.00      O
ATOM   2582  OW  WAT  1022       1.314  20.835   2.312  1.00 46.40      O
ATOM   2585  OW  WAT  1023       3.112  18.553   3.147  1.00 65.78      O
ATOM   2588  OW  WAT  1024      27.562   8.424  12.882  1.00 58.80      O
ATOM   2591  OW  WAT  1025      26.453   8.689  17.052  1.00 48.49      O
ATOM   2594  OW  WAT  1026       5.869  40.798  18.893  1.00 48.79      O
END
```

FIG. 6 CONT'D

FIG. 7 (TABLE 5)

Coordinates of hPR LBD in complex with R1881

	Nr.	Atom type	Molecule (hPR=dimeric)		Nr.	X	Y	Z			
ATOM	1	N	GLN	A	682	20.497	-20.862	-23.305	1.00	68.60	N
ATOM	2	CA	GLN	A	682	19.503	-21.064	-24.380	1.00	69.91	C
ATOM	3	C	GLN	A	682	18.229	-21.697	-23.807	1.00	68.48	C
ATOM	4	O	GLN	A	682	17.143	-21.664	-24.347	1.00	69.90	O
ATOM	5	CB	GLN	A	682	20.020	-21.875	-25.570	1.00	71.13	C
ATOM	6	N	LEU	A	683	18.368	-22.287	-22.640	1.00	66.32	N
ATOM	7	CA	LEU	A	683	17.309	-22.526	-21.704	1.00	62.77	C
ATOM	8	C	LEU	A	683	17.316	-21.477	-20.609	1.00	58.97	C
ATOM	9	O	LEU	A	683	16.249	-21.443	-20.021	1.00	55.97	O
ATOM	10	CB	LEU	A	683	17.498	-23.951	-21.162	1.00	65.72	C
ATOM	11	CG	LEU	A	683	16.409	-24.988	-21.409	1.00	67.24	C
ATOM	12	CD1	LEU	A	683	15.077	-24.271	-21.643	1.00	68.14	C
ATOM	13	CD2	LEU	A	683	16.692	-25.971	-22.539	1.00	68.46	C
ATOM	14	N	ILE	A	684	18.376	-20.707	-20.380	1.00	57.68	N
ATOM	15	CA	ILE	A	684	18.409	-19.708	-19.292	1.00	54.87	C
ATOM	16	C	ILE	A	684	17.729	-18.482	-19.894	1.00	51.46	C
ATOM	17	O	ILE	A	684	18.162	-18.002	-20.919	1.00	51.14	O
ATOM	18	CB	ILE	A	684	19.743	-19.375	-18.591	1.00	53.30	C
ATOM	19	CG1	ILE	A	684	20.378	-20.637	-17.959	1.00	51.27	C
ATOM	20	CG2	ILE	A	684	19.679	-18.330	-17.498	1.00	51.15	C
ATOM	21	CD1	ILE	A	684	19.366	-21.452	-17.179	1.00	50.03	C
ATOM	22	N	PRO	A	685	16.614	-18.156	-19.255	1.00	48.47	N
ATOM	23	CA	PRO	A	685	15.999	-16.875	-19.543	1.00	47.52	C
ATOM	24	C	PRO	A	685	16.988	-15.705	-19.389	1.00	46.96	C
ATOM	25	O	PRO	A	685	17.783	-15.551	-18.444	1.00	46.61	O
ATOM	26	CB	PRO	A	685	14.799	-16.934	-18.638	1.00	46.42	C
ATOM	27	CG	PRO	A	685	14.983	-17.997	-17.635	1.00	44.94	C
ATOM	28	CD	PRO	A	685	16.393	-18.437	-17.794	1.00	46.07	C
ATOM	29	N	PRO	A	686	16.875	-14.806	-20.397	1.00	44.87	N
ATOM	30	CA	PRO	A	686	17.893	-13.787	-20.636	1.00	42.14	C
ATOM	31	C	PRO	A	686	18.311	-12.833	-19.536	1.00	36.79	C
ATOM	32	O	PRO	A	686	19.517	-12.670	-19.427	1.00	34.82	O
ATOM	33	CB	PRO	A	686	17.467	-13.130	-21.943	1.00	42.03	C
ATOM	34	CG	PRO	A	686	16.624	-14.106	-22.644	1.00	41.43	C
ATOM	35	CD	PRO	A	686	16.208	-15.159	-21.694	1.00	42.48	C
ATOM	36	N	LEU	A	687	17.428	-12.322	-18.719	1.00	32.38	N
ATOM	37	CA	LEU	A	687	17.639	-11.687	-17.420	1.00	27.80	C
ATOM	38	C	LEU	A	687	18.448	-12.520	-16.455	1.00	26.34	C
ATOM	39	O	LEU	A	687	19.516	-12.105	-16.135	1.00	23.70	O
ATOM	40	CB	LEU	A	687	16.262	-11.320	-16.857	1.00	20.46	C
ATOM	41	CG	LEU	A	687	16.218	-10.278	-15.763	1.00	15.03	C
ATOM	42	CD1	LEU	A	687	17.167	-9.187	-16.281	1.00	10.95	C
ATOM	43	CD2	LEU	A	687	14.744	-10.067	-15.421	1.00	8.68	C
ATOM	44	N	ILE	A	688	18.135	-13.802	-16.326	1.00	28.10	N
ATOM	45	CA	ILE	A	688	18.865	-14.717	-15.455	1.00	27.04	C
ATOM	46	C	ILE	A	688	20.251	-14.728	-16.063	1.00	28.14	C
ATOM	47	O	ILE	A	688	21.106	-14.947	-15.202	1.00	28.63	O
ATOM	48	CB	ILE	A	688	18.238	-16.104	-15.281	1.00	22.58	C
ATOM	49	CG1	ILE	A	688	16.900	-16.103	-14.562	1.00	17.70	C
ATOM	50	CG2	ILE	A	688	19.220	-17.086	-14.614	1.00	21.80	C
ATOM	51	CD1	ILE	A	688	16.041	-17.279	-14.435	1.00	10.65	C
ATOM	52	N	ASN	A	689	20.606	-14.488	-17.305	1.00	27.48	N
ATOM	53	CA	ASN	A	689	21.989	-14.555	-17.661	1.00	29.03	C
ATOM	54	C	ASN	A	689	22.626	-13.207	-17.331	1.00	31.08	C
ATOM	55	O	ASN	A	689	23.821	-13.104	-17.132	1.00	28.02	O
ATOM	56	CB	ASN	A	689	22.326	-14.844	-19.077	1.00	30.30	C

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ATOM     57  CG  ASN A 689      21.783 -16.016 -19.851  1.00 32.25           C
ATOM     58  OD1 ASN A 689      21.438 -15.913 -21.064  1.00 28.32           O
ATOM     59  ND2 ASN A 689      21.758 -17.080 -19.032  1.00 31.87           N
ATOM     60  N   LEU A 690      21.802 -12.151 -17.384  1.00 33.58           N
ATOM     61  CA  LEU A 690      22.304 -10.825 -17.095  1.00 31.59           C
ATOM     62  C   LEU A 690      22.532 -10.821 -15.589  1.00 30.27           C
ATOM     63  O   LEU A 690      23.644 -10.480 -15.178  1.00 31.78           O
ATOM     64  CB  LEU A 690      21.470  -9.748 -17.782  1.00 29.77           C
ATOM     65  CG  LEU A 690      22.071  -8.314 -17.755  1.00 28.94           C
ATOM     66  CD1 LEU A 690      20.984  -7.416 -18.306  1.00 30.28           C
ATOM     67  CD2 LEU A 690      22.351  -7.693 -16.425  1.00 24.76           C
ATOM     68  N   LEU A 691      21.623 -11.247 -14.731  1.00 26.17           N
ATOM     69  CA  LEU A 691      21.914 -11.479 -13.339  1.00 23.77           C
ATOM     70  C   LEU A 691      23.263 -12.119 -13.152  1.00 25.57           C
ATOM     71  O   LEU A 691      24.224 -11.608 -12.585  1.00 24.09           O
ATOM     72  CB  LEU A 691      20.805 -12.213 -12.599  1.00 15.70           C
ATOM     73  CG  LEU A 691      19.475 -11.390 -12.510  1.00 12.57           C
ATOM     74  CD1 LEU A 691      18.532 -12.076 -11.475  1.00  9.03           C
ATOM     75  CD2 LEU A 691      19.629  -9.926 -12.273  1.00  7.87           C
ATOM     76  N   MET A 692      23.548 -13.267 -13.723  1.00 30.72           N
ATOM     77  CA  MET A 692      24.853 -13.889 -13.687  1.00 34.02           C
ATOM     78  C   MET A 692      25.930 -12.827 -13.804  1.00 35.93           C
ATOM     79  O   MET A 692      26.623 -12.545 -12.860  1.00 37.90           O
ATOM     80  CB  MET A 692      25.294 -14.924 -14.704  1.00 30.65           C
ATOM     81  CG  MET A 692      26.553 -15.665 -14.231  1.00 31.53           C
ATOM     82  SD  MET A 692      26.431 -16.866 -12.866  1.00 22.64           S
ATOM     83  CE  MET A 692      26.242 -15.633 -11.547  1.00 27.35           C
ATOM     84  N   SER A 693      25.969 -12.223 -14.998  1.00 37.17           N
ATOM     85  CA  SER A 693      27.066 -11.375 -15.437  1.00 32.44           C
ATOM     86  C   SER A 693      27.235 -10.197 -14.533  1.00 28.99           C
ATOM     87  O   SER A 693      28.388  -9.868 -14.374  1.00 26.65           O
ATOM     88  CB  SER A 693      27.172 -11.057 -16.905  1.00 28.75           C
ATOM     89  OG  SER A 693      26.151 -10.369 -17.490  1.00 26.83           O
ATOM     90  N   ILE A 694      26.219  -9.671 -13.923  1.00 28.58           N
ATOM     91  CA  ILE A 694      26.419  -8.388 -13.206  1.00 26.72           C
ATOM     92  C   ILE A 694      26.826  -8.702 -11.780  1.00 29.89           C
ATOM     93  O   ILE A 694      27.420  -7.804 -11.175  1.00 31.94           O
ATOM     94  CB  ILE A 694      25.270  -7.388 -13.267  1.00 20.16           C
ATOM     95  CG1 ILE A 694      23.895  -8.003 -13.143  1.00 17.56           C
ATOM     96  CG2 ILE A 694      25.348  -6.758 -14.660  1.00 17.15           C
ATOM     97  CD1 ILE A 694      22.940  -7.177 -12.352  1.00 17.17           C
ATOM     98  N   GLU A 695      26.602  -9.933 -11.326  1.00 31.55           N
ATOM     99  CA  GLU A 695      27.163 -10.359 -10.071  1.00 33.65           C
ATOM    100  C   GLU A 695      28.637  -9.932  -9.904  1.00 35.24           C
ATOM    101  O   GLU A 695      29.430 -10.234 -10.793  1.00 31.74           O
ATOM    102  CB  GLU A 695      27.030 -11.862  -9.864  1.00 33.91           C
ATOM    103  CG  GLU A 695      27.019 -12.393  -8.446  1.00 33.67           C
ATOM    104  CD  GLU A 695      25.821 -11.964  -7.599  1.00 33.90           C
ATOM    105  OE1 GLU A 695      24.849 -11.629  -8.297  1.00 34.22           O
ATOM    106  OE2 GLU A 695      25.842 -11.998  -6.336  1.00 34.61           O
ATOM    107  N   PRO A 696      28.896  -9.274  -8.757  1.00 37.14           N
ATOM    108  CA  PRO A 696      30.174  -8.821  -8.351  1.00 38.49           C
ATOM    109  C   PRO A 696      31.264  -9.846  -8.296  1.00 39.84           C
ATOM    110  O   PRO A 696      30.955 -10.950  -7.908  1.00 40.66           O
ATOM    111  CB  PRO A 696      29.912  -8.420  -6.881  1.00 38.71           C
ATOM    112  CG  PRO A 696      28.489  -8.164  -6.660  1.00 37.76           C
ATOM    113  CD  PRO A 696      27.821  -8.879  -7.801  1.00 37.06           C
ATOM    114  N   ASP A 697      32.532  -9.551  -8.496  1.00 42.18           N
ATOM    115  CA  ASP A 697      33.638 -10.421  -8.087  1.00 44.28           C
ATOM    116  C   ASP A 697      34.026 -10.470  -6.588  1.00 43.77           C
ATOM    117  O   ASP A 697      33.644  -9.624  -5.798  1.00 42.94           O
ATOM    118  CB  ASP A 697      34.835 -10.151  -9.023  1.00 44.65           C
ATOM    119  CG  ASP A 697      35.964 -11.138  -8.728  1.00 46.43           C
ATOM    120  OD1 ASP A 697      35.641 -12.305  -8.359  1.00 45.33           O
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FIG. 7 CONT'D

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ATOM    121  OD2 ASP A 697      37.195 -10.777  -8.776  1.00 47.86           O
ATOM    122  N   VAL A 698      34.732 -11.485  -6.087  1.00 42.66           N
ATOM    123  CA  VAL A 698      34.729 -11.890  -4.698  1.00 41.90           C
ATOM    124  C   VAL A 698      35.408 -10.749  -3.989  1.00 38.79           C
ATOM    125  O   VAL A 698      36.330 -10.224  -4.588  1.00 40.04           O
ATOM    126  CB  VAL A 698      35.521 -13.163  -4.366  1.00 43.54           C
ATOM    127  CG1 VAL A 698      35.880 -13.981  -5.625  1.00 42.69           C
ATOM    128  CG2 VAL A 698      36.799 -12.937  -3.546  1.00 42.88           C
ATOM    129  N   ILE A 699      34.986 -10.416  -2.811  1.00 34.60           N
ATOM    130  CA  ILE A 699      35.551  -9.350  -1.991  1.00 28.63           C
ATOM    131  C   ILE A 699      36.288 -10.009  -0.814  1.00 29.19           C
ATOM    132  O   ILE A 699      35.709 -10.746  -0.008  1.00 27.50           O
ATOM    133  CB  ILE A 699      34.428  -8.512  -1.343  1.00 22.03           C
ATOM    134  CG1 ILE A 699      33.378  -7.998  -2.264  1.00 19.01           C
ATOM    135  CG2 ILE A 699      34.955  -7.478  -0.392  1.00 18.81           C
ATOM    136  CD1 ILE A 699      33.573  -7.023  -3.406  1.00 16.09           C
ATOM    137  N   TYR A 700      37.551  -9.724  -0.698  1.00 30.13           N
ATOM    138  CA  TYR A 700      38.331 -10.071   0.488  1.00 33.03           C
ATOM    139  C   TYR A 700      38.056  -9.107   1.612  1.00 33.35           C
ATOM    140  O   TYR A 700      37.349  -8.119   1.539  1.00 34.67           O
ATOM    141  CB  TYR A 700      39.811 -10.231   0.139  1.00 32.40           C
ATOM    142  CG  TYR A 700      40.141 -11.116  -1.037  1.00 33.77           C
ATOM    143  CD1 TYR A 700      39.554 -10.926  -2.293  1.00 35.06           C
ATOM    144  CD2 TYR A 700      41.056 -12.143  -1.024  1.00 33.85           C
ATOM    145  CE1 TYR A 700      39.794 -11.688  -3.407  1.00 34.38           C
ATOM    146  CE2 TYR A 700      41.337 -12.943  -2.112  1.00 33.60           C
ATOM    147  CZ  TYR A 700      40.712 -12.722  -3.306  1.00 35.80           C
ATOM    148  OH  TYR A 700      40.924 -13.499  -4.453  1.00 36.08           O
ATOM    149  N   ALA A 701      38.356  -9.469   2.825  1.00 35.57           N
ATOM    150  CA  ALA A 701      38.288  -8.698   4.041  1.00 37.77           C
ATOM    151  C   ALA A 701      39.577  -7.949   4.311  1.00 39.69           C
ATOM    152  O   ALA A 701      39.518  -7.022   5.074  1.00 37.84           O
ATOM    153  CB  ALA A 701      37.910  -9.580   5.194  1.00 36.13           C
ATOM    154  N   GLY A 702      40.676  -8.308   3.691  1.00 42.24           N
ATOM    155  CA  GLY A 702      41.983  -7.801   4.038  1.00 49.06           C
ATOM    156  C   GLY A 702      42.362  -8.041   5.490  1.00 54.18           C
ATOM    157  O   GLY A 702      42.863  -7.097   6.090  1.00 54.26           O
ATOM    158  N   HIS A 703      42.187  -9.231   6.009  1.00 59.06           N
ATOM    159  CA  HIS A 703      42.112  -9.575   7.406  1.00 62.94           C
ATOM    160  C   HIS A 703      43.455 -10.142   7.851  1.00 66.96           C
ATOM    161  O   HIS A 703      44.011 -10.956   7.093  1.00 68.30           O
ATOM    162  CB  HIS A 703      40.927 -10.578   7.424  1.00 60.90           C
ATOM    163  CG  HIS A 703      40.822 -11.171   8.778  1.00 61.65           C
ATOM    164  ND1 HIS A 703      41.330 -12.415   9.057  1.00 62.29           N
ATOM    165  CD2 HIS A 703      40.375 -10.656   9.942  1.00 61.87           C
ATOM    166  CE1 HIS A 703      41.159 -12.656  10.358  1.00 62.49           C
ATOM    167  NE2 HIS A 703      40.570 -11.599  10.913  1.00 62.37           N
ATOM    168  N   ASP A 704      44.019  -9.724   8.993  1.00 66.77           N
ATOM    169  CA  ASP A 704      45.455  -9.904   9.234  1.00 68.11           C
ATOM    170  C   ASP A 704      45.855 -11.355   9.409  1.00 70.35           C
ATOM    171  O   ASP A 704      46.999 -11.716   9.060  1.00 69.89           O
ATOM    172  CB  ASP A 704      46.025  -8.984  10.324  1.00 65.16           C
ATOM    173  N   ASN A 705      45.047 -12.280   9.880  1.00 73.46           N
ATOM    174  CA  ASN A 705      45.140 -13.725   9.966  1.00 76.00           C
ATOM    175  C   ASN A 705      46.404 -14.175  10.705  1.00 76.76           C
ATOM    176  O   ASN A 705      46.305 -14.992  11.643  1.00 76.87           O
ATOM    177  CB  ASN A 705      44.903 -14.564   8.684  1.00 75.23           C
ATOM    178  N   THR A 706      47.567 -13.683  10.312  1.00 77.29           N
ATOM    179  CA  THR A 706      48.698 -13.564  11.202  1.00 79.23           C
ATOM    180  C   THR A 706      48.337 -13.873  12.660  1.00 79.97           C
ATOM    181  O   THR A 706      48.386 -15.029  13.112  1.00 79.74           O
ATOM    182  CB  THR A 706      49.274 -12.130  11.177  1.00 78.70           C
ATOM    183  N   LYS A 707      47.949 -12.775  13.342  1.00 80.02           N
ATOM    184  CA  LYS A 707      47.909 -12.895  14.802  1.00 80.91           C
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FIG. 7 CONT'D

ATOM	185	C	LYS	A	707	46.490	-13.087	15.333	1.00	80.69	C
ATOM	186	O	LYS	A	707	45.458	-12.722	14.778	1.00	80.86	O
ATOM	187	CB	LYS	A	707	48.720	-11.801	15.507	1.00	80.59	C
ATOM	188	N	PRO	A	708	46.472	-13.718	16.517	1.00	79.87	N
ATOM	189	CA	PRO	A	708	45.304	-14.284	17.134	1.00	78.95	C
ATOM	190	C	PRO	A	708	44.117	-13.364	17.331	1.00	77.53	C
ATOM	191	O	PRO	A	708	44.119	-12.418	18.124	1.00	76.83	O
ATOM	192	CB	PRO	A	708	45.809	-14.678	18.528	1.00	80.40	C
ATOM	193	CG	PRO	A	708	46.762	-13.563	18.855	1.00	81.32	C
ATOM	194	CD	PRO	A	708	47.516	-13.383	17.559	1.00	80.83	C
ATOM	195	N	ASP	A	709	43.048	-13.744	16.627	1.00	75.99	N
ATOM	196	CA	ASP	A	709	41.762	-13.060	16.694	1.00	73.61	C
ATOM	197	C	ASP	A	709	41.526	-12.456	18.077	1.00	71.22	C
ATOM	198	O	ASP	A	709	41.590	-13.217	19.046	1.00	72.96	O
ATOM	199	CB	ASP	A	709	40.563	-13.969	16.373	1.00	71.95	C
ATOM	200	CG	ASP	A	709	40.527	-14.324	14.909	1.00	71.44	C
ATOM	201	OD1	ASP	A	709	41.440	-13.850	14.203	1.00	71.02	O
ATOM	202	OD2	ASP	A	709	39.598	-15.060	14.514	1.00	71.54	O
ATOM	203	N	THR	A	710	41.278	-11.168	18.241	1.00	66.66	N
ATOM	204	CA	THR	A	710	40.527	-10.811	19.466	1.00	61.19	C
ATOM	205	C	THR	A	710	39.103	-10.535	19.046	1.00	58.34	C
ATOM	206	O	THR	A	710	38.844	-10.672	17.848	1.00	55.95	O
ATOM	207	CB	THR	A	710	41.242	-9.735	20.245	1.00	59.73	C
ATOM	208	OG1	THR	A	710	40.255	-8.750	20.567	1.00	60.16	O
ATOM	209	CG2	THR	A	710	42.414	-9.153	19.486	1.00	58.68	C
ATOM	210	N	SER	A	711	38.188	-10.261	19.951	1.00	56.31	N
ATOM	211	CA	SER	A	711	36.800	-10.139	19.455	1.00	54.49	C
ATOM	212	C	SER	A	711	36.542	-8.780	18.856	1.00	53.30	C
ATOM	213	O	SER	A	711	35.840	-8.707	17.855	1.00	53.41	O
ATOM	214	CB	SER	A	711	35.848	-10.702	20.476	1.00	53.77	C
ATOM	215	OG	SER	A	711	35.900	-12.146	20.461	1.00	51.95	O
ATOM	216	N	SER	A	712	37.257	-7.726	19.198	1.00	51.12	N
ATOM	217	CA	SER	A	712	37.295	-6.438	18.543	1.00	48.87	C
ATOM	218	C	SER	A	712	37.897	-6.395	17.147	1.00	47.44	C
ATOM	219	O	SER	A	712	37.363	-5.754	16.204	1.00	47.78	O
ATOM	220	CB	SER	A	712	38.172	-5.601	19.488	1.00	49.96	C
ATOM	221	OG	SER	A	712	39.129	-6.572	19.916	1.00	50.83	O
ATOM	222	N	SER	A	713	38.998	-7.157	16.980	1.00	43.47	N
ATOM	223	CA	SER	A	713	39.633	-7.231	15.647	1.00	38.31	C
ATOM	224	C	SER	A	713	38.814	-7.894	14.511	1.00	33.85	C
ATOM	225	O	SER	A	713	38.811	-7.518	13.355	1.00	30.14	O
ATOM	226	CB	SER	A	713	40.990	-7.884	15.756	1.00	36.08	C
ATOM	227	OG	SER	A	713	41.077	-9.114	15.025	1.00	39.33	O
ATOM	228	N	LEU	A	714	38.137	-8.969	14.846	1.00	30.62	N
ATOM	229	CA	LEU	A	714	37.228	-9.689	14.084	1.00	29.96	C
ATOM	230	C	LEU	A	714	36.060	-8.799	13.694	1.00	29.91	C
ATOM	231	O	LEU	A	714	35.751	-8.663	12.523	1.00	28.31	O
ATOM	232	CB	LEU	A	714	36.799	-10.888	14.880	1.00	28.31	C
ATOM	233	CG	LEU	A	714	36.703	-12.267	14.200	1.00	27.47	C
ATOM	234	CD1	LEU	A	714	37.715	-12.287	13.053	1.00	26.94	C
ATOM	235	CD2	LEU	A	714	36.947	-13.504	15.076	1.00	23.27	C
ATOM	236	N	LEU	A	715	35.404	-8.183	14.644	1.00	28.31	N
ATOM	237	CA	LEU	A	715	34.402	-7.177	14.509	1.00	23.92	C
ATOM	238	C	LEU	A	715	34.870	-6.077	13.619	1.00	24.97	C
ATOM	239	O	LEU	A	715	34.182	-5.729	12.663	1.00	25.92	O
ATOM	240	CB	LEU	A	715	33.946	-6.701	15.905	1.00	19.35	C
ATOM	241	CG	LEU	A	715	32.850	-7.656	16.375	1.00	17.12	C
ATOM	242	CD1	LEU	A	715	31.596	-6.970	16.945	1.00	17.68	C
ATOM	243	CD2	LEU	A	715	32.220	-8.571	15.262	1.00	13.48	C
ATOM	244	N	THR	A	716	36.040	-5.547	13.867	1.00	25.03	N
ATOM	245	CA	THR	A	716	36.595	-4.602	12.894	1.00	25.65	C
ATOM	246	C	THR	A	716	36.833	-5.128	11.536	1.00	25.52	C
ATOM	247	O	THR	A	716	36.732	-4.364	10.583	1.00	28.47	O
ATOM	248	CB	THR	A	716	37.887	-4.009	13.507	1.00	24.12	C

FIG. 7 CONT'D

ATOM	249	OG1	THR	A	716	37.212	-3.167	14.462	1.00	25.08	O
ATOM	250	CG2	THR	A	716	38.874	-3.219	12.700	1.00	17.25	C
ATOM	251	N	SER	A	717	37.292	-6.312	11.276	1.00	26.43	N
ATOM	252	CA	SER	A	717	37.461	-6.852	9.915	1.00	26.06	C
ATOM	253	C	SER	A	717	36.150	-7.012	9.180	1.00	24.95	C
ATOM	254	O	SER	A	717	35.843	-6.416	8.156	1.00	24.11	O
ATOM	255	CB	SER	A	717	38.146	-8.198	10.011	1.00	23.71	C
ATOM	256	OG	SER	A	717	39.355	-8.024	9.344	1.00	22.07	O
ATOM	257	N	LEU	A	718	35.221	-7.630	9.899	1.00	23.80	N
ATOM	258	CA	LEU	A	718	33.872	-7.765	9.469	1.00	23.64	C
ATOM	259	C	LEU	A	718	33.395	-6.470	8.821	1.00	25.44	C
ATOM	260	O	LEU	A	718	32.661	-6.488	7.823	1.00	26.14	O
ATOM	261	CB	LEU	A	718	33.050	-8.482	10.526	1.00	18.81	C
ATOM	262	CG	LEU	A	718	33.081	-10.041	10.421	1.00	17.19	C
ATOM	263	CD1	LEU	A	718	31.976	-10.692	11.229	1.00	16.62	C
ATOM	264	CD2	LEU	A	718	32.963	-10.677	9.046	1.00	15.35	C
ATOM	265	N	ASN	A	719	33.686	-5.318	9.369	1.00	23.12	N
ATOM	266	CA	ASN	A	719	33.142	-4.061	9.031	1.00	18.50	C
ATOM	267	C	ASN	A	719	33.787	-3.634	7.744	1.00	20.25	C
ATOM	268	O	ASN	A	719	33.149	-3.246	6.768	1.00	20.49	O
ATOM	269	CB	ASN	A	719	33.631	-3.236	10.199	1.00	10.77	C
ATOM	270	CG	ASN	A	719	32.499	-3.163	11.168	1.00	7.59	C
ATOM	271	OD1	ASN	A	719	31.510	-3.775	10.809	1.00	8.73	O
ATOM	272	ND2	ASN	A	719	32.598	-2.426	12.294	1.00	7.41	N
ATOM	273	N	GLN	A	720	35.107	-3.766	7.759	1.00	20.13	N
ATOM	274	CA	GLN	A	720	35.916	-3.306	6.634	1.00	17.48	C
ATOM	275	C	GLN	A	720	35.405	-4.100	5.478	1.00	19.58	C
ATOM	276	O	GLN	A	720	35.155	-3.652	4.408	1.00	14.45	O
ATOM	277	CB	GLN	A	720	37.349	-3.621	6.809	1.00	13.68	C
ATOM	278	CG	GLN	A	720	38.386	-3.358	5.826	1.00	15.34	C
ATOM	279	CD	GLN	A	720	38.503	-2.025	5.211	1.00	21.39	C
ATOM	280	OE1	GLN	A	720	38.719	-1.028	5.974	1.00	27.38	O
ATOM	281	NE2	GLN	A	720	38.390	-1.939	3.913	1.00	19.66	N
ATOM	282	N	LEU	A	721	35.241	-5.437	5.770	1.00	22.47	N
ATOM	283	CA	LEU	A	721	34.643	-6.324	4.798	1.00	19.53	C
ATOM	284	C	LEU	A	721	33.256	-5.872	4.325	1.00	19.21	C
ATOM	285	O	LEU	A	721	32.976	-5.780	3.144	1.00	14.91	O
ATOM	286	CB	LEU	A	721	34.869	-7.690	5.402	1.00	14.72	C
ATOM	287	CG	LEU	A	721	34.160	-8.545	4.334	1.00	17.28	C
ATOM	288	CD1	LEU	A	721	35.251	-8.965	3.392	1.00	17.60	C
ATOM	289	CD2	LEU	A	721	33.228	-9.651	4.713	1.00	15.03	C
ATOM	290	N	GLY	A	722	32.334	-5.429	5.113	1.00	19.34	N
ATOM	291	CA	GLY	A	722	31.062	-4.808	4.998	1.00	21.01	C
ATOM	292	C	GLY	A	722	31.112	-3.518	4.175	1.00	23.69	C
ATOM	293	O	GLY	A	722	30.435	-3.467	3.116	1.00	23.83	O
ATOM	294	N	GLU	A	723	31.971	-2.560	4.548	1.00	21.10	N
ATOM	295	CA	GLU	A	723	32.322	-1.509	3.639	1.00	19.31	C
ATOM	296	C	GLU	A	723	32.566	-1.971	2.220	1.00	21.70	C
ATOM	297	O	GLU	A	723	31.898	-1.593	1.304	1.00	22.30	O
ATOM	298	CB	GLU	A	723	33.482	-0.686	4.113	1.00	15.61	C
ATOM	299	CG	GLU	A	723	33.729	0.718	3.707	1.00	13.72	C
ATOM	300	CD	GLU	A	723	32.817	1.836	4.168	1.00	11.15	C
ATOM	301	OE1	GLU	A	723	31.739	1.367	4.551	1.00	3.23	O
ATOM	302	OE2	GLU	A	723	33.292	3.032	4.131	1.00	9.08	O
ATOM	303	N	ARG	A	724	33.415	-2.885	1.861	1.00	24.30	N
ATOM	304	CA	ARG	A	724	33.807	-3.322	0.560	1.00	22.79	C
ATOM	305	C	ARG	A	724	32.630	-4.017	-0.119	1.00	23.13	C
ATOM	306	O	ARG	A	724	32.514	-3.973	-1.319	1.00	23.31	O
ATOM	307	CB	ARG	A	724	35.070	-4.116	0.517	1.00	18.29	C
ATOM	308	CG	ARG	A	724	36.426	-3.551	0.885	1.00	16.48	C
ATOM	309	CD	ARG	A	724	36.800	-4.035	2.245	1.00	22.18	C
ATOM	310	NE	ARG	A	724	38.114	-4.080	2.849	1.00	24.53	N
ATOM	311	CZ	ARG	A	724	39.196	-4.667	2.341	1.00	22.88	C
ATOM	312	NH1	ARG	A	724	39.010	-5.289	1.174	1.00	23.48	N

FIG. 7 CONT'D

ATOM	313	NH2	ARG	A	724	40.394	-4.671	2.831	1.00	20.72	N
ATOM	314	N	GLN	A	725	31.672	-4.486	0.621	1.00	22.71	N
ATOM	315	CA	GLN	A	725	30.532	-5.144	0.102	1.00	21.76	C
ATOM	316	C	GLN	A	725	29.470	-4.106	-0.179	1.00	22.01	C
ATOM	317	O	GLN	A	725	28.683	-4.474	-1.037	1.00	25.25	O
ATOM	318	CB	GLN	A	725	29.908	-6.241	0.970	1.00	17.02	C
ATOM	319	CG	GLN	A	725	30.723	-7.506	0.993	1.00	12.59	C
ATOM	320	CD	GLN	A	725	30.004	-8.658	1.643	1.00	11.30	C
ATOM	321	OE1	GLN	A	725	28.957	-8.516	2.235	1.00	9.65	O
ATOM	322	NE2	GLN	A	725	30.558	-9.842	1.502	1.00	9.72	N
ATOM	323	N	LEU	A	726	29.360	-2.978	0.438	1.00	18.32	N
ATOM	324	CA	LEU	A	726	28.335	-1.987	0.104	1.00	12.01	C
ATOM	325	C	LEU	A	726	28.744	-1.154	-1.087	1.00	12.64	C
ATOM	326	O	LEU	A	726	27.940	-0.770	-1.917	1.00	2.86	O
ATOM	327	CB	LEU	A	726	28.368	-1.254	1.414	1.00	2.02	C
ATOM	328	CG	LEU	A	726	27.369	-0.122	1.736	1.00	4.91	C
ATOM	329	CD1	LEU	A	726	25.930	-0.633	1.341	1.00	2.02	C
ATOM	330	CD2	LEU	A	726	27.534	0.602	3.095	1.00	2.02	C
ATOM	331	N	LEU	A	727	30.010	-0.861	-1.316	1.00	14.66	N
ATOM	332	CA	LEU	A	727	30.487	-0.408	-2.606	1.00	18.62	C
ATOM	333	C	LEU	A	727	30.077	-1.415	-3.707	1.00	22.69	C
ATOM	334	O	LEU	A	727	29.503	-1.081	-4.808	1.00	24.47	O
ATOM	335	CB	LEU	A	727	31.960	0.029	-2.656	1.00	16.94	C
ATOM	336	CG	LEU	A	727	32.563	0.629	-3.951	1.00	12.89	C
ATOM	337	CD1	LEU	A	727	32.251	2.102	-4.040	1.00	15.29	C
ATOM	338	CD2	LEU	A	727	34.060	0.486	-4.164	1.00	8.42	C
ATOM	339	N	SER	A	728	30.202	-2.722	-3.454	1.00	21.01	N
ATOM	340	CA	SER	A	728	29.927	-3.691	-4.479	1.00	18.46	C
ATOM	341	C	SER	A	728	28.429	-3.736	-4.707	1.00	16.89	C
ATOM	342	O	SER	A	728	27.906	-3.956	-5.843	1.00	13.50	O
ATOM	343	CB	SER	A	728	30.666	-4.972	-4.162	1.00	17.61	C
ATOM	344	OG	SER	A	728	31.447	-5.575	-5.180	1.00	17.47	O
ATOM	345	N	VAL	A	729	27.634	-3.512	-3.685	1.00	14.62	N
ATOM	346	CA	VAL	A	729	26.199	-3.355	-3.919	1.00	12.68	C
ATOM	347	C	VAL	A	729	25.764	-2.108	-4.701	1.00	11.52	C
ATOM	348	O	VAL	A	729	24.730	-2.168	-5.461	1.00	5.27	O
ATOM	349	CB	VAL	A	729	25.431	-3.482	-2.606	1.00	11.20	C
ATOM	350	CG1	VAL	A	729	24.066	-2.822	-2.688	1.00	11.41	C
ATOM	351	CG2	VAL	A	729	25.386	-4.990	-2.400	1.00	8.44	C
ATOM	352	N	VAL	A	730	26.538	-1.025	-4.531	1.00	5.12	N
ATOM	353	CA	VAL	A	730	26.138	0.100	-5.346	1.00	10.35	C
ATOM	354	C	VAL	A	730	26.474	-0.117	-6.787	1.00	15.32	C
ATOM	355	O	VAL	A	730	25.674	-0.029	-7.672	1.00	14.88	O
ATOM	356	CB	VAL	A	730	26.612	1.388	-4.674	1.00	2.91	C
ATOM	357	CG1	VAL	A	730	25.658	2.500	-5.147	1.00	6.98	C
ATOM	358	CG2	VAL	A	730	26.398	1.129	-3.180	1.00	9.15	C
ATOM	359	N	LYS	A	731	27.700	-0.583	-7.016	1.00	21.50	N
ATOM	360	CA	LYS	A	731	28.044	-0.915	-8.396	1.00	22.93	C
ATOM	361	C	LYS	A	731	27.030	-1.864	-9.018	1.00	21.79	C
ATOM	362	O	LYS	A	731	26.740	-1.693	-10.191	1.00	21.51	O
ATOM	363	CB	LYS	A	731	29.446	-1.437	-8.595	1.00	19.96	C
ATOM	364	CG	LYS	A	731	30.488	-0.650	-7.938	1.00	22.98	C
ATOM	365	CD	LYS	A	731	31.743	-0.219	-8.608	1.00	26.11	C
ATOM	366	CE	LYS	A	731	32.568	-1.071	-9.526	1.00	25.56	C
ATOM	367	NZ	LYS	A	731	31.803	-1.730	-10.578	1.00	25.76	N
ATOM	368	N	TRP	A	732	26.629	-2.881	-8.243	1.00	18.52	N
ATOM	369	CA	TRP	A	732	25.779	-3.968	-8.696	1.00	16.31	C
ATOM	370	C	TRP	A	732	24.431	-3.313	-9.042	1.00	14.47	C
ATOM	371	O	TRP	A	732	24.122	-3.449	-10.190	1.00	12.38	O
ATOM	372	CB	TRP	A	732	25.519	-5.319	-7.971	1.00	13.57	C
ATOM	373	CG	TRP	A	732	24.379	-6.331	-8.170	1.00	7.50	C
ATOM	374	CD1	TRP	A	732	24.254	-7.361	-9.084	1.00	2.02	C
ATOM	375	CD2	TRP	A	732	23.144	-6.323	-7.429	1.00	6.38	C
ATOM	376	NE1	TRP	A	732	23.071	-7.948	-8.788	1.00	5.86	N

FIG. 7 CONT'D

ATOM	377	CE2	TRP	A	732	22.285	-7.387	-7.864	1.00	2.02	C
ATOM	378	CE3	TRP	A	732	22.682	-5.467	-6.420	1.00	2.02	C
ATOM	379	CZ2	TRP	A	732	21.049	-7.607	-7.312	1.00	4.17	C
ATOM	380	CZ3	TRP	A	732	21.474	-5.754	-5.853	1.00	6.75	C
ATOM	381	CH2	TRP	A	732	20.628	-6.811	-6.312	1.00	5.13	C
ATOM	382	N	SER	A	733	23.815	-2.643	-8.123	1.00	15.45	N
ATOM	383	CA	SER	A	733	22.614	-1.907	-8.445	1.00	15.59	C
ATOM	384	C	SER	A	733	22.624	-1.045	-9.716	1.00	14.71	C
ATOM	385	O	SER	A	733	21.649	-1.259	-10.488	1.00	2.84	O
ATOM	386	CB	SER	A	733	22.114	-1.285	-7.148	1.00	2.02	C
ATOM	387	OG	SER	A	733	22.545	0.021	-7.253	1.00	2.84	O
ATOM	388	N	LYS	A	734	23.660	-0.378	-10.153	1.00	14.87	N
ATOM	389	CA	LYS	A	734	23.771	0.481	-11.295	1.00	17.69	C
ATOM	390	C	LYS	A	734	23.663	-0.305	-12.619	1.00	18.19	C
ATOM	391	O	LYS	A	734	23.240	0.173	-13.669	1.00	17.63	O
ATOM	392	CB	LYS	A	734	25.022	1.363	-11.339	1.00	19.29	C
ATOM	393	CG	LYS	A	734	25.655	1.983	-10.110	1.00	20.14	C
ATOM	394	CD	LYS	A	734	25.673	3.518	-10.060	1.00	21.00	C
ATOM	395	CE	LYS	A	734	26.835	3.888	-10.988	1.00	22.10	C
ATOM	396	NZ	LYS	A	734	27.562	5.061	-10.491	1.00	21.32	N
ATOM	397	N	SER	A	735	23.859	-1.578	-12.770	1.00	15.34	N
ATOM	398	CA	SER	A	735	23.598	-2.403	-13.841	1.00	12.89	C
ATOM	399	C	SER	A	735	22.365	-3.295	-13.743	1.00	14.36	C
ATOM	400	O	SER	A	735	22.228	-4.196	-14.601	1.00	13.55	O
ATOM	401	CB	SER	A	735	24.759	-3.399	-13.997	1.00	10.83	C
ATOM	402	OG	SER	A	735	25.874	-2.732	-14.393	1.00	8.49	O
ATOM	403	N	LEU	A	736	21.563	-3.179	-12.745	1.00	14.51	N
ATOM	404	CA	LEU	A	736	20.518	-4.220	-12.612	1.00	16.56	C
ATOM	405	C	LEU	A	736	19.306	-3.594	-13.306	1.00	20.19	C
ATOM	406	O	LEU	A	736	18.957	-2.395	-13.243	1.00	20.02	O
ATOM	407	CB	LEU	A	736	20.441	-4.542	-11.138	1.00	10.74	C
ATOM	408	CG	LEU	A	736	19.082	-5.087	-10.779	1.00	10.44	C
ATOM	409	CD1	LEU	A	736	19.289	-6.537	-11.107	1.00	9.58	C
ATOM	410	CD2	LEU	A	736	18.586	-4.786	-9.392	1.00	8.25	C
ATOM	411	N	PRO	A	737	18.726	-4.418	-14.201	1.00	19.84	N
ATOM	412	CA	PRO	A	737	17.696	-3.887	-15.132	1.00	16.74	C
ATOM	413	C	PRO	A	737	16.542	-3.268	-14.423	1.00	15.37	C
ATOM	414	O	PRO	A	737	15.994	-3.796	-13.491	1.00	19.86	O
ATOM	415	CB	PRO	A	737	17.534	-5.127	-16.023	1.00	11.83	C
ATOM	416	CG	PRO	A	737	18.921	-5.499	-16.248	1.00	10.50	C
ATOM	417	CD	PRO	A	737	19.277	-5.695	-14.757	1.00	15.10	C
ATOM	418	N	GLY	A	738	16.170	-2.028	-14.556	1.00	15.43	N
ATOM	419	CA	GLY	A	738	15.148	-1.356	-13.812	1.00	15.35	C
ATOM	420	C	GLY	A	738	15.593	-0.583	-12.628	1.00	18.36	C
ATOM	421	O	GLY	A	738	14.993	0.451	-12.551	1.00	21.09	O
ATOM	422	N	PHE	A	739	16.568	-0.920	-11.781	1.00	19.63	N
ATOM	423	CA	PHE	A	739	16.963	-0.147	-10.626	1.00	18.59	C
ATOM	424	C	PHE	A	739	17.148	1.318	-10.985	1.00	17.07	C
ATOM	425	O	PHE	A	739	16.468	2.116	-10.368	1.00	14.69	O
ATOM	426	CB	PHE	A	739	18.059	-0.800	-9.697	1.00	15.65	C
ATOM	427	CG	PHE	A	739	17.979	-0.398	-8.236	1.00	10.38	C
ATOM	428	CD1	PHE	A	739	16.901	-0.646	-7.429	1.00	8.41	C
ATOM	429	CD2	PHE	A	739	18.995	0.343	-7.681	1.00	9.40	C
ATOM	430	CE1	PHE	A	739	16.778	-0.227	-6.115	1.00	8.74	C
ATOM	431	CE2	PHE	A	739	18.907	0.741	-6.353	1.00	10.45	C
ATOM	432	CZ	PHE	A	739	17.801	0.452	-5.549	1.00	9.21	C
ATOM	433	N	ARG	A	740	17.847	1.679	-12.020	1.00	18.47	N
ATOM	434	CA	ARG	A	740	18.164	3.088	-12.230	1.00	19.40	C
ATOM	435	C	ARG	A	740	17.040	3.919	-12.807	1.00	21.61	C
ATOM	436	O	ARG	A	740	17.368	5.007	-13.202	1.00	21.47	O
ATOM	437	CB	ARG	A	740	19.288	3.412	-13.253	1.00	13.18	C
ATOM	438	CG	ARG	A	740	18.825	2.732	-14.550	1.00	9.52	C
ATOM	439	CD	ARG	A	740	19.951	2.700	-15.511	1.00	8.43	C
ATOM	440	NE	ARG	A	740	19.643	2.131	-16.825	1.00	8.39	N

FIG. 7 CONT'D

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ATOM    441  CZ  ARG A 740      20.349   2.609 -17.881  1.00  6.83           C
ATOM    442  NH1 ARG A 740      21.240   3.555 -17.702  1.00  4.10           N
ATOM    443  NH2 ARG A 740      20.043   2.159 -19.053  1.00  6.19           N
ATOM    444  N   ASN A 741      15.834   3.475 -13.011  1.00 24.60           N
ATOM    445  CA  ASN A 741      14.763   4.246 -13.539  1.00 23.95           C
ATOM    446  C   ASN A 741      13.812   4.471 -12.390  1.00 24.11           C
ATOM    447  O   ASN A 741      12.808   5.072 -12.684  1.00 24.48           O
ATOM    448  CB  ASN A 741      14.027   3.525 -14.689  1.00 23.21           C
ATOM    449  CG  ASN A 741      14.758   2.717 -15.691  1.00 17.90           C
ATOM    450  OD1 ASN A 741      14.314   1.807 -16.340  1.00 18.14           O
ATOM    451  ND2 ASN A 741      16.042   2.969 -15.872  1.00 19.01           N
ATOM    452  N   LEU A 742      14.095   3.968 -11.185  1.00 24.78           N
ATOM    453  CA  LEU A 742      13.546   4.697  -9.995  1.00 22.52           C
ATOM    454  C   LEU A 742      14.320   5.996  -9.751  1.00 21.89           C
ATOM    455  O   LEU A 742      15.426   6.364 -10.118  1.00 16.77           O
ATOM    456  CB  LEU A 742      13.383   3.766  -8.853  1.00 20.13           C
ATOM    457  CG  LEU A 742      12.991   2.294  -8.884  1.00 19.35           C
ATOM    458  CD1 LEU A 742      13.863   1.421  -7.976  1.00 17.90           C
ATOM    459  CD2 LEU A 742      11.536   2.279  -8.398  1.00 19.38           C
ATOM    460  N   HIS A 743      13.629   6.947  -9.176  1.00 25.53           N
ATOM    461  CA  HIS A 743      14.150   8.171  -8.545  1.00 29.70           C
ATOM    462  C   HIS A 743      15.340   7.986  -7.608  1.00 29.55           C
ATOM    463  O   HIS A 743      15.359   7.099  -6.711  1.00 30.80           O
ATOM    464  CB  HIS A 743      12.884   8.799  -7.940  1.00 30.56           C
ATOM    465  CG  HIS A 743      13.064  10.249  -7.691  1.00 32.71           C
ATOM    466  ND1 HIS A 743      13.706  10.633  -6.509  1.00 34.24           N
ATOM    467  CD2 HIS A 743      12.773  11.340  -8.387  1.00 32.55           C
ATOM    468  CE1 HIS A 743      13.832  11.969  -6.497  1.00 34.27           C
ATOM    469  NE2 HIS A 743      13.270  12.397  -7.589  1.00 34.91           N
ATOM    470  N   ILE A 744      16.409   8.777  -7.777  1.00 27.13           N
ATOM    471  CA  ILE A 744      17.615   8.694  -6.996  1.00 27.03           C
ATOM    472  C   ILE A 744      17.371   8.237  -5.541  1.00 27.39           C
ATOM    473  O   ILE A 744      18.088   7.396  -5.031  1.00 26.32           O
ATOM    474  CB  ILE A 744      18.572   9.911  -6.797  1.00 24.86           C
ATOM    475  CG1 ILE A 744      19.543  10.048  -7.985  1.00 24.02           C
ATOM    476  CG2 ILE A 744      19.560   9.939  -5.631  1.00 20.02           C
ATOM    477  CD1 ILE A 744      19.806   8.740  -8.653  1.00 24.17           C
ATOM    478  N   ASP A 745      16.517   8.930  -4.870  1.00 27.06           N
ATOM    479  CA  ASP A 745      16.128   8.839  -3.517  1.00 26.45           C
ATOM    480  C   ASP A 745      15.812   7.447  -2.984  1.00 23.69           C
ATOM    481  O   ASP A 745      16.136   6.867  -1.980  1.00 22.63           O
ATOM    482  CB  ASP A 745      14.787   9.639  -3.429  1.00 27.97           C
ATOM    483  CG  ASP A 745      14.976  11.065  -2.945  1.00 28.60           C
ATOM    484  OD1 ASP A 745      16.123  11.439  -2.706  1.00 26.49           O
ATOM    485  OD2 ASP A 745      14.021  11.886  -2.833  1.00 29.28           O
ATOM    486  N   ASP A 746      14.841   6.901  -3.588  1.00 20.28           N
ATOM    487  CA  ASP A 746      14.312   5.618  -3.640  1.00 20.23           C
ATOM    488  C   ASP A 746      15.348   4.520  -3.825  1.00 21.38           C
ATOM    489  O   ASP A 746      15.326   3.448  -3.242  1.00 21.79           O
ATOM    490  CB  ASP A 746      13.306   5.836  -4.823  1.00 15.44           C
ATOM    491  CG  ASP A 746      12.037   6.428  -4.199  1.00 11.66           C
ATOM    492  OD1 ASP A 746      12.099   7.101  -3.150  1.00 10.95           O
ATOM    493  OD2 ASP A 746      10.938   6.155  -4.669  1.00  2.66           O
ATOM    494  N   GLN A 747      16.323   4.673  -4.693  1.00 21.30           N
ATOM    495  CA  GLN A 747      17.496   3.882  -4.890  1.00 18.22           C
ATOM    496  C   GLN A 747      18.429   3.988  -3.697  1.00 19.43           C
ATOM    497  O   GLN A 747      19.049   2.968  -3.369  1.00 20.04           O
ATOM    498  CB  GLN A 747      18.312   4.423  -6.083  1.00 11.65           C
ATOM    499  CG  GLN A 747      17.682   4.132  -7.380  1.00  2.11           C
ATOM    500  CD  GLN A 747      18.295   4.780  -8.651  1.00  7.28           C
ATOM    501  OE1 GLN A 747      17.717   5.400  -9.626  1.00  4.60           O
ATOM    502  NE2 GLN A 747      19.595   4.740  -8.944  1.00  4.19           N
ATOM    503  N   ILE A 748      18.606   5.187  -3.149  1.00 18.06           N
ATOM    504  CA  ILE A 748      19.230   5.351  -1.864  1.00 17.21           C
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FIG. 7 CONT'D

ATOM	505	C	ILE	A	748	18.453	4.727	-0.679	1.00	17.44	C
ATOM	506	O	ILE	A	748	19.120	4.050	0.076	1.00	18.75	O
ATOM	507	CB	ILE	A	748	19.529	6.772	-1.440	1.00	13.51	C
ATOM	508	CG1	ILE	A	748	20.261	7.560	-2.506	1.00	10.74	C
ATOM	509	CG2	ILE	A	748	20.399	6.809	-0.189	1.00	10.90	C
ATOM	510	CD1	ILE	A	748	19.796	8.960	-2.154	1.00	8.83	C
ATOM	511	N	THR	A	749	17.171	4.963	-0.509	1.00	15.58	N
ATOM	512	CA	THR	A	749	16.393	4.265	0.472	1.00	13.04	C
ATOM	513	C	THR	A	749	16.441	2.789	0.373	1.00	14.88	C
ATOM	514	O	THR	A	749	16.861	2.224	1.392	1.00	14.95	O
ATOM	515	CB	THR	A	749	14.896	4.660	0.574	1.00	2.57	C
ATOM	516	OG1	THR	A	749	14.940	6.033	0.268	1.00	7.12	O
ATOM	517	CG2	THR	A	749	14.314	3.965	1.789	1.00	7.39	C
ATOM	518	N	LEU	A	750	16.109	2.093	-0.700	1.00	15.47	N
ATOM	519	CA	LEU	A	750	16.178	0.624	-0.784	1.00	11.53	C
ATOM	520	C	LEU	A	750	17.597	0.085	-0.555	1.00	11.11	C
ATOM	521	O	LEU	A	750	17.627	-0.934	0.124	1.00	11.00	O
ATOM	522	CB	LEU	A	750	15.654	0.039	-2.070	1.00	2.02	C
ATOM	523	CG	LEU	A	750	14.357	0.698	-2.602	1.00	7.94	C
ATOM	524	CD1	LEU	A	750	14.007	0.757	-4.124	1.00	8.42	C
ATOM	525	CD2	LEU	A	750	13.099	0.189	-1.912	1.00	5.51	C
ATOM	526	N	ILE	A	751	18.679	0.699	-1.051	1.00	9.20	N
ATOM	527	CA	ILE	A	751	19.926	0.087	-0.552	1.00	8.85	C
ATOM	528	C	ILE	A	751	20.096	0.253	0.929	1.00	8.54	C
ATOM	529	O	ILE	A	751	20.138	-0.629	1.689	1.00	6.25	O
ATOM	530	CB	ILE	A	751	20.945	0.756	-1.473	1.00	4.54	C
ATOM	531	CG1	ILE	A	751	20.768	0.267	-2.923	1.00	6.55	C
ATOM	532	CG2	ILE	A	751	22.233	0.619	-0.698	1.00	3.22	C
ATOM	533	CD1	ILE	A	751	21.787	0.794	-3.945	1.00	3.14	C
ATOM	534	N	GLN	A	752	20.040	1.371	1.584	1.00	11.53	N
ATOM	535	CA	GLN	A	752	20.171	1.734	2.947	1.00	13.09	C
ATOM	536	C	GLN	A	752	19.303	0.695	3.683	1.00	13.71	C
ATOM	537	O	GLN	A	752	19.966	0.073	4.514	1.00	14.02	O
ATOM	538	CB	GLN	A	752	19.812	3.126	3.470	1.00	6.54	C
ATOM	539	CG	GLN	A	752	20.982	4.032	3.282	1.00	2.02	C
ATOM	540	CD	GLN	A	752	20.571	5.471	2.977	1.00	5.25	C
ATOM	541	OE1	GLN	A	752	19.545	6.097	2.697	1.00	2.99	O
ATOM	542	NE2	GLN	A	752	21.813	5.997	2.886	1.00	4.67	N
ATOM	543	N	TYR	A	753	18.085	0.527	3.331	1.00	12.34	N
ATOM	544	CA	TYR	A	753	17.242	-0.498	3.844	1.00	11.23	C
ATOM	545	C	TYR	A	753	17.510	-1.934	3.467	1.00	10.57	C
ATOM	546	O	TYR	A	753	16.873	-2.748	4.089	1.00	9.05	O
ATOM	547	CB	TYR	A	753	15.838	-0.278	3.245	1.00	11.75	C
ATOM	548	CG	TYR	A	753	15.004	0.865	3.860	1.00	10.57	C
ATOM	549	CD1	TYR	A	753	15.588	1.977	4.576	1.00	2.02	C
ATOM	550	CD2	TYR	A	753	13.643	0.709	3.534	1.00	8.26	C
ATOM	551	CE1	TYR	A	753	14.586	2.830	4.996	1.00	5.35	C
ATOM	552	CE2	TYR	A	753	12.758	1.677	4.005	1.00	7.61	C
ATOM	553	CZ	TYR	A	753	13.229	2.734	4.756	1.00	3.25	C
ATOM	554	OH	TYR	A	753	12.237	3.615	5.115	1.00	6.86	O
ATOM	555	N	SER	A	754	18.322	-2.423	2.581	1.00	12.55	N
ATOM	556	CA	SER	A	754	18.551	-3.857	2.450	1.00	13.43	C
ATOM	557	C	SER	A	754	19.963	-4.395	2.769	1.00	13.33	C
ATOM	558	O	SER	A	754	20.226	-5.546	2.311	1.00	9.24	O
ATOM	559	CB	SER	A	754	18.193	-4.432	1.032	1.00	11.29	C
ATOM	560	OG	SER	A	754	18.511	-3.392	0.089	1.00	6.27	O
ATOM	561	N	TRP	A	755	20.882	-3.624	3.329	1.00	15.01	N
ATOM	562	CA	TRP	A	755	22.275	-3.999	2.997	1.00	21.88	C
ATOM	563	C	TRP	A	755	22.559	-5.166	3.947	1.00	23.20	C
ATOM	564	O	TRP	A	755	23.038	-6.177	3.514	1.00	21.71	O
ATOM	565	CB	TRP	A	755	23.217	-2.810	2.952	1.00	22.83	C
ATOM	566	CG	TRP	A	755	23.146	-2.278	4.370	1.00	28.61	C
ATOM	567	CD1	TRP	A	755	22.084	-1.592	4.928	1.00	30.09	C
ATOM	568	CD2	TRP	A	755	24.121	-2.523	5.411	1.00	27.83	C

FIG. 7 CONT'D

ATOM	569	NE1	TRP	A	755	22.353	-1.377	6.254	1.00	32.01	N
ATOM	570	CE2	TRP	A	755	23.591	-1.908	6.565	1.00	29.68	C
ATOM	571	CE3	TRP	A	755	25.361	-3.116	5.406	1.00	25.52	C
ATOM	572	CZ2	TRP	A	755	24.238	-1.891	7.780	1.00	29.85	C
ATOM	573	CZ3	TRP	A	755	26.019	-3.102	6.588	1.00	28.82	C
ATOM	574	CH2	TRP	A	755	25.467	-2.490	7.739	1.00	30.89	C
ATOM	575	N	MET	A	756	22.257	-5.025	5.253	1.00	21.71	N
ATOM	576	CA	MET	A	756	22.261	-6.176	6.090	1.00	17.72	C
ATOM	577	C	MET	A	756	21.687	-7.397	5.313	1.00	15.06	C
ATOM	578	O	MET	A	756	22.416	-8.372	5.178	1.00	13.21	O
ATOM	579	CB	MET	A	756	21.487	-5.857	7.359	1.00	10.45	C
ATOM	580	CG	MET	A	756	21.905	-6.966	8.313	1.00	7.34	C
ATOM	581	SD	MET	A	756	23.684	-6.725	8.600	1.00	10.08	S
ATOM	582	CE	MET	A	756	23.737	-5.383	9.855	1.00	7.48	C
ATOM	583	N	SER	A	757	20.458	-7.392	4.901	1.00	12.75	N
ATOM	584	CA	SER	A	757	19.731	-8.545	4.443	1.00	12.53	C
ATOM	585	C	SER	A	757	20.369	-9.143	3.185	1.00	14.38	C
ATOM	586	O	SER	A	757	20.697	-10.331	3.073	1.00	12.95	O
ATOM	587	CB	SER	A	757	18.327	-8.085	4.440	1.00	9.68	C
ATOM	588	OG	SER	A	757	17.253	-8.876	4.027	1.00	13.18	O
ATOM	589	N	LEU	A	758	20.868	-8.397	2.265	1.00	13.15	N
ATOM	590	CA	LEU	A	758	21.834	-8.717	1.291	1.00	12.65	C
ATOM	591	C	LEU	A	758	23.166	-9.295	1.616	1.00	17.62	C
ATOM	592	O	LEU	A	758	23.584	-10.112	0.769	1.00	23.36	O
ATOM	593	CB	LEU	A	758	21.995	-7.407	0.613	1.00	2.02	C
ATOM	594	CG	LEU	A	758	20.942	-6.879	-0.405	1.00	3.99	C
ATOM	595	CD1	LEU	A	758	21.597	-5.938	-1.387	1.00	5.68	C
ATOM	596	CD2	LEU	A	758	20.332	-8.055	-1.127	1.00	3.36	C
ATOM	597	N	MET	A	759	24.048	-8.951	2.479	1.00	19.05	N
ATOM	598	CA	MET	A	759	25.180	-9.361	3.146	1.00	18.31	C
ATOM	599	C	MET	A	759	24.945	-10.751	3.752	1.00	19.93	C
ATOM	600	O	MET	A	759	25.694	-11.743	3.588	1.00	19.60	O
ATOM	601	CB	MET	A	759	25.402	-8.489	4.361	1.00	14.92	C
ATOM	602	CG	MET	A	759	25.626	-7.022	4.371	1.00	15.45	C
ATOM	603	SD	MET	A	759	27.135	-6.354	5.153	1.00	15.53	S
ATOM	604	CE	MET	A	759	27.422	-5.156	3.782	1.00	20.41	C
ATOM	605	N	VAL	A	760	23.830	-10.763	4.482	1.00	19.13	N
ATOM	606	CA	VAL	A	760	23.527	-12.062	5.130	1.00	19.01	C
ATOM	607	C	VAL	A	760	23.192	-13.214	4.223	1.00	20.30	C
ATOM	608	O	VAL	A	760	23.592	-14.341	4.236	1.00	19.65	O
ATOM	609	CB	VAL	A	760	22.587	-11.740	6.297	1.00	13.91	C
ATOM	610	CG1	VAL	A	760	21.103	-11.853	6.104	1.00	11.30	C
ATOM	611	CG2	VAL	A	760	23.122	-12.664	7.367	1.00	13.35	C
ATOM	612	N	PHE	A	761	22.353	-13.050	3.252	1.00	22.16	N
ATOM	613	CA	PHE	A	761	21.953	-13.814	2.120	1.00	22.18	C
ATOM	614	C	PHE	A	761	23.067	-14.462	1.307	1.00	22.67	C
ATOM	615	O	PHE	A	761	22.963	-15.602	0.859	1.00	22.08	O
ATOM	616	CB	PHE	A	761	21.159	-13.031	1.058	1.00	16.30	C
ATOM	617	CG	PHE	A	761	20.271	-13.934	0.281	1.00	12.34	C
ATOM	618	CD1	PHE	A	761	19.486	-14.873	0.968	1.00	8.15	C
ATOM	619	CD2	PHE	A	761	20.228	-13.834	-1.133	1.00	9.09	C
ATOM	620	CE1	PHE	A	761	18.579	-15.654	0.248	1.00	7.63	C
ATOM	621	CE2	PHE	A	761	19.359	-14.687	-1.809	1.00	6.15	C
ATOM	622	CZ	PHE	A	761	18.502	-15.525	-1.170	1.00	3.59	C
ATOM	623	N	GLY	A	762	24.100	-13.742	1.023	1.00	22.78	N
ATOM	624	CA	GLY	A	762	25.178	-14.135	0.157	1.00	20.41	C
ATOM	625	C	GLY	A	762	26.276	-14.695	0.983	1.00	20.83	C
ATOM	626	O	GLY	A	762	27.099	-15.438	0.507	1.00	21.81	O
ATOM	627	N	LEU	A	763	26.411	-14.347	2.261	1.00	22.96	N
ATOM	628	CA	LEU	A	763	27.144	-15.199	3.174	1.00	19.44	C
ATOM	629	C	LEU	A	763	26.396	-16.535	3.097	1.00	20.10	C
ATOM	630	O	LEU	A	763	26.990	-17.511	2.680	1.00	17.59	O
ATOM	631	CB	LEU	A	763	27.183	-14.524	4.509	1.00	11.39	C
ATOM	632	CG	LEU	A	763	27.621	-15.521	5.641	1.00	8.96	C

FIG. 7 CONT'D

ATOM	633	CD1	LEU	A	763	29.083	-15.487	5.971	1.00	2.95	C
ATOM	634	CD2	LEU	A	763	26.565	-15.505	6.742	1.00	2.94	C
ATOM	635	N	GLY	A	764	25.139	-16.711	3.415	1.00	19.89	N
ATOM	636	CA	GLY	A	764	24.434	-17.907	3.034	1.00	21.45	C
ATOM	637	C	GLY	A	764	24.960	-18.610	1.779	1.00	22.78	C
ATOM	638	O	GLY	A	764	25.414	-19.730	1.657	1.00	22.23	O
ATOM	639	N	TRP	A	765	24.771	-18.011	0.618	1.00	21.70	N
ATOM	640	CA	TRP	A	765	24.996	-18.417	-0.692	1.00	17.95	C
ATOM	641	C	TRP	A	765	26.410	-18.950	-0.660	1.00	19.59	C
ATOM	642	O	TRP	A	765	26.682	-20.142	-0.795	1.00	20.55	O
ATOM	643	CB	TRP	A	765	24.607	-17.376	-1.770	1.00	10.74	C
ATOM	644	CG	TRP	A	765	25.091	-17.864	-3.128	1.00	5.12	C
ATOM	645	CD1	TRP	A	765	26.256	-17.629	-3.840	1.00	2.51	C
ATOM	646	CD2	TRP	A	765	24.447	-18.968	-3.798	1.00	5.02	C
ATOM	647	NE1	TRP	A	765	26.396	-18.537	-4.877	1.00	6.28	N
ATOM	648	CE2	TRP	A	765	25.240	-19.252	-4.931	1.00	7.80	C
ATOM	649	CE3	TRP	A	765	23.227	-19.672	-3.615	1.00	4.08	C
ATOM	650	CZ2	TRP	A	765	24.824	-20.206	-5.872	1.00	10.10	C
ATOM	651	CZ3	TRP	A	765	22.851	-20.713	-4.473	1.00	5.41	C
ATOM	652	CH2	TRP	A	765	23.696	-20.998	-5.564	1.00	8.02	C
ATOM	653	N	ARG	A	766	27.352	-18.059	-0.544	1.00	21.52	N
ATOM	654	CA	ARG	A	766	28.761	-18.432	-0.562	1.00	22.87	C
ATOM	655	C	ARG	A	766	29.123	-19.468	0.503	1.00	23.84	C
ATOM	656	O	ARG	A	766	30.178	-20.066	0.336	1.00	26.05	O
ATOM	657	CB	ARG	A	766	29.644	-17.206	-0.384	1.00	18.43	C
ATOM	658	CG	ARG	A	766	30.017	-16.203	-1.357	1.00	14.30	C
ATOM	659	CD	ARG	A	766	31.091	-15.181	-1.026	1.00	13.11	C
ATOM	660	NE	ARG	A	766	30.892	-14.429	0.188	1.00	10.97	N
ATOM	661	CZ	ARG	A	766	30.091	-13.475	0.625	1.00	10.89	C
ATOM	662	NH1	ARG	A	766	29.153	-12.920	-0.172	1.00	7.92	N
ATOM	663	NH2	ARG	A	766	30.251	-13.085	1.919	1.00	12.76	N
ATOM	664	N	SER	A	767	28.440	-19.634	1.612	1.00	23.87	N
ATOM	665	CA	SER	A	767	28.774	-20.626	2.609	1.00	24.76	C
ATOM	666	C	SER	A	767	28.396	-22.035	2.122	1.00	29.53	C
ATOM	667	O	SER	A	767	29.207	-22.977	2.176	1.00	28.81	O
ATOM	668	CB	SER	A	767	28.184	-20.177	3.963	1.00	18.14	C
ATOM	669	OG	SER	A	767	29.231	-19.259	4.344	1.00	14.34	O
ATOM	670	N	TYR	A	768	27.162	-22.035	1.608	1.00	30.95	N
ATOM	671	CA	TYR	A	768	26.601	-23.125	0.858	1.00	31.59	C
ATOM	672	C	TYR	A	768	27.442	-23.477	-0.329	1.00	31.06	C
ATOM	673	O	TYR	A	768	27.713	-24.640	-0.429	1.00	32.11	O
ATOM	674	CB	TYR	A	768	25.170	-22.727	0.469	1.00	32.87	C
ATOM	675	CG	TYR	A	768	24.338	-23.633	-0.409	1.00	32.54	C
ATOM	676	CD1	TYR	A	768	23.960	-24.912	-0.097	1.00	32.35	C
ATOM	677	CD2	TYR	A	768	23.933	-23.216	-1.658	1.00	31.91	C
ATOM	678	CE1	TYR	A	768	23.229	-25.712	-0.943	1.00	32.34	C
ATOM	679	CE2	TYR	A	768	23.220	-23.968	-2.547	1.00	31.49	C
ATOM	680	CZ	TYR	A	768	22.855	-25.233	-2.167	1.00	31.92	C
ATOM	681	OH	TYR	A	768	22.136	-26.014	-3.031	1.00	28.89	O
ATOM	682	N	LYS	A	769	27.883	-22.644	-1.183	1.00	31.77	N
ATOM	683	CA	LYS	A	769	28.644	-23.038	-2.322	1.00	35.15	C
ATOM	684	C	LYS	A	769	30.013	-23.572	-2.023	1.00	36.76	C
ATOM	685	O	LYS	A	769	30.320	-24.465	-2.826	1.00	38.69	O
ATOM	686	CB	LYS	A	769	28.941	-21.858	-3.265	1.00	33.90	C
ATOM	687	CG	LYS	A	769	28.264	-21.924	-4.593	1.00	30.70	C
ATOM	688	CD	LYS	A	769	28.908	-22.649	-5.718	1.00	29.03	C
ATOM	689	CE	LYS	A	769	28.003	-22.858	-6.918	1.00	28.94	C
ATOM	690	NZ	LYS	A	769	28.436	-23.528	-8.188	1.00	23.59	N
ATOM	691	N	HIS	A	770	30.875	-23.008	-1.187	1.00	35.13	N
ATOM	692	CA	HIS	A	770	32.218	-23.544	-1.164	1.00	33.96	C
ATOM	693	C	HIS	A	770	32.584	-24.281	0.108	1.00	33.23	C
ATOM	694	O	HIS	A	770	33.730	-24.755	0.180	1.00	33.94	O
ATOM	695	CB	HIS	A	770	33.387	-22.639	-1.403	1.00	34.78	C
ATOM	696	CG	HIS	A	770	33.385	-21.350	-2.134	1.00	35.01	C

FIG. 7 CONT'D

ATOM	697	ND1	HIS	A	770	34.210	-21.216	-3.239	1.00	33.96	N
ATOM	698	CD2	HIS	A	770	32.804	-20.159	-2.016	1.00	34.42	C
ATOM	699	CE1	HIS	A	770	34.165	-20.064	-3.772	1.00	31.27	C
ATOM	700	NE2	HIS	A	770	33.312	-19.426	-3.026	1.00	33.97	N
ATOM	701	N	VAL	A	771	31.857	-24.378	1.169	1.00	30.68	N
ATOM	702	CA	VAL	A	771	32.314	-25.067	2.358	1.00	27.91	C
ATOM	703	C	VAL	A	771	31.111	-25.893	2.852	1.00	30.04	C
ATOM	704	O	VAL	A	771	30.926	-26.006	4.047	1.00	30.99	O
ATOM	705	CB	VAL	A	771	32.842	-24.331	3.583	1.00	20.97	C
ATOM	706	CG1	VAL	A	771	34.311	-23.980	3.386	1.00	18.93	C
ATOM	707	CG2	VAL	A	771	31.950	-23.195	4.060	1.00	15.92	C
ATOM	708	N	SER	A	772	30.255	-26.312	1.968	1.00	28.43	N
ATOM	709	CA	SER	A	772	29.173	-27.180	2.200	1.00	27.75	C
ATOM	710	C	SER	A	772	28.145	-26.731	3.187	1.00	31.61	C
ATOM	711	O	SER	A	772	27.434	-27.593	3.665	1.00	32.99	O
ATOM	712	CB	SER	A	772	29.614	-28.580	2.572	1.00	22.25	C
ATOM	713	OG	SER	A	772	29.993	-29.417	1.532	1.00	12.79	O
ATOM	714	N	GLY	A	773	28.045	-25.431	3.474	1.00	34.18	N
ATOM	715	CA	GLY	A	773	27.195	-24.815	4.482	1.00	32.43	C
ATOM	716	C	GLY	A	773	27.690	-25.121	5.902	1.00	31.00	C
ATOM	717	O	GLY	A	773	27.030	-25.003	6.929	1.00	28.10	O
ATOM	718	N	GLN	A	774	28.913	-25.602	6.027	1.00	31.21	N
ATOM	719	CA	GLN	A	774	29.430	-26.144	7.284	1.00	31.14	C
ATOM	720	C	GLN	A	774	30.418	-25.233	8.006	1.00	29.93	C
ATOM	721	O	GLN	A	774	31.028	-25.619	8.968	1.00	30.99	O
ATOM	722	CB	GLN	A	774	29.820	-27.575	6.836	1.00	27.97	C
ATOM	723	CG	GLN	A	774	29.107	-28.744	7.478	1.00	24.91	C
ATOM	724	CD	GLN	A	774	27.603	-28.536	7.502	1.00	26.66	C
ATOM	725	OE1	GLN	A	774	27.046	-28.653	8.607	1.00	24.02	O
ATOM	726	NE2	GLN	A	774	26.984	-28.229	6.308	1.00	24.78	N
ATOM	727	N	MET	A	775	30.709	-24.017	7.671	1.00	27.13	N
ATOM	728	CA	MET	A	775	31.613	-23.011	8.007	1.00	23.89	C
ATOM	729	C	MET	A	775	31.033	-21.713	7.442	1.00	21.39	C
ATOM	730	O	MET	A	775	30.473	-21.991	6.416	1.00	19.79	O
ATOM	731	CB	MET	A	775	33.019	-23.003	7.379	1.00	21.79	C
ATOM	732	CG	MET	A	775	33.800	-24.250	7.712	1.00	16.88	C
ATOM	733	SD	MET	A	775	35.488	-24.032	8.201	1.00	15.28	S
ATOM	734	CE	MET	A	775	36.157	-25.684	8.073	1.00	17.52	C
ATOM	735	N	LEU	A	776	31.181	-20.537	8.007	1.00	19.39	N
ATOM	736	CA	LEU	A	776	30.674	-19.288	7.500	1.00	15.78	C
ATOM	737	C	LEU	A	776	31.714	-18.614	6.615	1.00	20.15	C
ATOM	738	O	LEU	A	776	32.772	-18.285	7.058	1.00	20.51	O
ATOM	739	CB	LEU	A	776	30.283	-18.325	8.578	1.00	2.02	C
ATOM	740	CG	LEU	A	776	29.083	-18.844	9.362	1.00	3.77	C
ATOM	741	CD1	LEU	A	776	28.719	-17.763	10.425	1.00	3.10	C
ATOM	742	CD2	LEU	A	776	27.868	-18.975	8.546	1.00	3.67	C
ATOM	743	N	TYR	A	777	31.408	-18.479	5.317	1.00	22.32	N
ATOM	744	CA	TYR	A	777	32.380	-18.035	4.338	1.00	23.31	C
ATOM	745	C	TYR	A	777	32.157	-16.546	4.099	1.00	25.08	C
ATOM	746	O	TYR	A	777	31.736	-16.229	3.011	1.00	25.41	O
ATOM	747	CB	TYR	A	777	32.092	-18.764	3.038	1.00	20.16	C
ATOM	748	CG	TYR	A	777	33.263	-18.762	2.089	1.00	16.61	C
ATOM	749	CD1	TYR	A	777	34.299	-19.647	2.297	1.00	15.29	CD2 C
ATOM	750	CD2	TYR	A	777	33.301	-17.898	1.023	1.00	13.89	CD1 C
ATOM	751	CE1	TYR	A	777	35.382	-19.606	1.455	1.00	13.89	CE2 C
ATOM	752	CE2	TYR	A	777	34.354	-17.916	0.145	1.00	12.08	CE1 C
ATOM	753	CZ	TYR	A	777	35.392	-18.760	0.395	1.00	11.74	C
ATOM	754	OH	TYR	A	777	36.442	-18.856	-0.449	1.00	11.45	O
ATOM	755	N	PHE	A	778	32.300	-15.703	5.126	1.00	23.69	N
ATOM	756	CA	PHE	A	778	32.485	-14.291	4.982	1.00	22.33	C
ATOM	757	C	PHE	A	778	33.271	-13.786	3.760	1.00	23.15	C
ATOM	758	O	PHE	A	778	32.771	-12.988	3.009	1.00	23.28	O
ATOM	759	CB	PHE	A	778	32.935	-13.640	6.327	1.00	13.72	C
ATOM	760	CG	PHE	A	778	31.774	-13.570	7.284	1.00	2.02	C

FIG. 7 CONT'D

ATOM	761	CD1	PHE	A	778	30.747	-12.759	7.533	1.00	7.56	CD2 C
ATOM	762	CD2	PHE	A	778	31.850	-14.572	8.291	1.00	6.69	CD1 C
ATOM	763	CE1	PHE	A	778	29.803	-13.009	8.541	1.00	8.16	CE2 C
ATOM	764	CE2	PHE	A	778	30.920	-14.869	9.216	1.00	2.02	CE1 C
ATOM	765	CZ	PHE	A	778	29.880	-14.030	9.399	1.00	6.23	C
ATOM	766	N	ALA	A	779	34.457	-14.172	3.444	1.00	22.75	N
ATOM	767	CA	ALA	A	779	35.382	-13.947	2.414	1.00	20.37	C
ATOM	768	C	ALA	A	779	36.433	-15.030	2.291	1.00	20.96	C
ATOM	769	O	ALA	A	779	36.796	-15.809	3.171	1.00	16.54	O
ATOM	770	CB	ALA	A	779	36.045	-12.571	2.632	1.00	16.42	C
ATOM	771	N	PRO	A	780	37.070	-15.084	1.127	1.00	23.79	N
ATOM	772	CA	PRO	A	780	38.185	-16.001	0.910	1.00	26.85	C
ATOM	773	C	PRO	A	780	39.180	-15.900	2.044	1.00	29.66	C
ATOM	774	O	PRO	A	780	39.698	-16.894	2.505	1.00	33.32	O
ATOM	775	CB	PRO	A	780	38.714	-15.645	-0.461	1.00	22.38	C
ATOM	776	CG	PRO	A	780	37.779	-14.684	-1.051	1.00	20.37	C
ATOM	777	CD	PRO	A	780	36.527	-14.779	-0.221	1.00	20.93	C
ATOM	778	N	ASP	A	781	39.627	-14.769	2.459	1.00	30.45	N
ATOM	779	CA	ASP	A	781	40.478	-14.498	3.575	1.00	29.90	C
ATOM	780	C	ASP	A	781	39.795	-14.367	4.921	1.00	28.26	C
ATOM	781	O	ASP	A	781	40.535	-14.081	5.861	1.00	30.65	O
ATOM	782	CB	ASP	A	781	41.268	-13.241	3.155	1.00	28.23	C
ATOM	783	CG	ASP	A	781	40.231	-12.144	3.131	1.00	26.56	C
ATOM	784	OD1	ASP	A	781	39.093	-12.391	2.725	1.00	27.71	O
ATOM	785	OD2	ASP	A	781	40.481	-11.023	3.550	1.00	27.46	O
ATOM	786	N	LEU	A	782	38.535	-14.595	5.069	1.00	24.91	N
ATOM	787	CA	LEU	A	782	37.894	-14.714	6.327	1.00	24.29	C
ATOM	788	C	LEU	A	782	36.802	-15.774	6.408	1.00	24.16	C
ATOM	789	O	LEU	A	782	35.658	-15.459	6.133	1.00	22.18	O
ATOM	790	CB	LEU	A	782	37.426	-13.300	6.762	1.00	17.60	C
ATOM	791	CG	LEU	A	782	36.885	-13.348	8.248	1.00	12.48	C
ATOM	792	CD1	LEU	A	782	37.922	-14.128	9.101	1.00	2.02	C
ATOM	793	CD2	LEU	A	782	36.415	-11.995	8.632	1.00	6.46	C
ATOM	794	N	ILE	A	783	37.115	-17.014	6.818	1.00	26.06	N
ATOM	795	CA	ILE	A	783	36.221	-18.167	6.934	1.00	26.79	C
ATOM	796	C	ILE	A	783	35.882	-18.642	8.312	1.00	28.73	C
ATOM	797	O	ILE	A	783	36.788	-19.266	8.798	1.00	32.02	O
ATOM	798	CB	ILE	A	783	36.603	-19.493	6.221	1.00	22.16	C
ATOM	799	CG1	ILE	A	783	36.692	-19.243	4.734	1.00	20.70	C
ATOM	800	CG2	ILE	A	783	35.505	-20.543	6.372	1.00	21.03	C
ATOM	801	CD1	ILE	A	783	37.653	-19.909	3.858	1.00	20.99	C
ATOM	802	N	LEU	A	784	34.779	-18.577	8.985	1.00	31.38	N
ATOM	803	CA	LEU	A	784	34.705	-18.933	10.392	1.00	34.42	C
ATOM	804	C	LEU	A	784	34.171	-20.326	10.635	1.00	37.18	C
ATOM	805	O	LEU	A	784	33.015	-20.607	10.407	1.00	37.85	O
ATOM	806	CB	LEU	A	784	33.884	-17.977	11.263	1.00	29.24	C
ATOM	807	CG	LEU	A	784	34.340	-16.547	11.293	1.00	26.38	C
ATOM	808	CD1	LEU	A	784	33.626	-15.801	12.398	1.00	27.85	C
ATOM	809	CD2	LEU	A	784	35.834	-16.430	11.459	1.00	26.53	C
ATOM	810	N	ASN	A	785	35.023	-21.160	11.204	1.00	42.21	N
ATOM	811	CA	ASN	A	785	34.591	-22.433	11.804	1.00	45.50	C
ATOM	812	C	ASN	A	785	34.219	-22.266	13.297	1.00	45.96	C
ATOM	813	O	ASN	A	785	34.135	-21.156	13.813	1.00	43.41	O
ATOM	814	CB	ASN	A	785	35.603	-23.543	11.727	1.00	42.79	C
ATOM	815	CG	ASN	A	785	36.904	-23.075	12.339	1.00	43.59	C
ATOM	816	OD1	ASN	A	785	37.135	-22.351	13.298	1.00	40.82	O
ATOM	817	ND2	ASN	A	785	37.865	-23.631	11.590	1.00	45.30	N
ATOM	818	N	GLU	A	786	33.862	-23.389	13.916	1.00	48.69	N
ATOM	819	CA	GLU	A	786	33.209	-23.437	15.208	1.00	51.15	C
ATOM	820	C	GLU	A	786	34.120	-23.035	16.376	1.00	52.76	C
ATOM	821	O	GLU	A	786	33.801	-22.538	17.444	1.00	53.65	O
ATOM	822	CB	GLU	A	786	32.887	-24.866	15.607	1.00	50.56	C
ATOM	823	CG	GLU	A	786	31.440	-25.282	15.573	1.00	52.86	C
ATOM	824	CD	GLU	A	786	30.871	-25.016	14.165	1.00	53.44	C

FIG. 7 CONT'D

ATOM	825	OE1	GLU	A	786	31.399	-25.555	13.171	1.00	51.13	O
ATOM	826	OE2	GLU	A	786	29.915	-24.213	14.225	1.00	52.78	O
ATOM	827	N	GLN	A	787	35.372	-23.420	16.229	1.00	53.33	N
ATOM	828	CA	GLN	A	787	36.504	-23.043	17.012	1.00	52.92	C
ATOM	829	C	GLN	A	787	36.364	-21.532	17.120	1.00	55.00	C
ATOM	830	O	GLN	A	787	35.660	-20.935	17.937	1.00	56.93	O
ATOM	831	CB	GLN	A	787	37.833	-23.371	16.389	1.00	50.86	C
ATOM	832	CG	GLN	A	787	38.699	-24.543	16.488	1.00	53.17	C
ATOM	833	CD	GLN	A	787	38.499	-26.032	16.620	1.00	54.85	C
ATOM	834	OE1	GLN	A	787	39.314	-26.848	17.142	1.00	52.24	O
ATOM	835	NE2	GLN	A	787	37.397	-26.672	16.166	1.00	55.90	N
ATOM	836	N	ARG	A	788	37.053	-20.837	16.236	1.00	54.53	N
ATOM	837	CA	ARG	A	788	36.890	-19.423	15.960	1.00	52.71	C
ATOM	838	C	ARG	A	788	35.699	-18.623	16.432	1.00	50.80	C
ATOM	839	O	ARG	A	788	35.967	-17.419	16.766	1.00	50.55	O
ATOM	840	CB	ARG	A	788	37.170	-19.213	14.451	1.00	52.60	C
ATOM	841	CG	ARG	A	788	38.663	-19.399	14.178	1.00	53.66	C
ATOM	842	CD	ARG	A	788	39.074	-18.788	12.860	1.00	55.36	C
ATOM	843	NE	ARG	A	788	39.466	-17.370	12.873	1.00	54.35	N
ATOM	844	CZ	ARG	A	788	39.678	-16.665	11.756	1.00	53.16	C
ATOM	845	NH1	ARG	A	788	39.564	-17.196	10.531	1.00	51.67	N
ATOM	846	NH2	ARG	A	788	39.985	-15.406	12.043	1.00	51.42	N
ATOM	847	N	MET	A	789	34.443	-18.993	16.638	1.00	48.65	N
ATOM	848	CA	MET	A	789	33.465	-18.104	17.273	1.00	46.37	C
ATOM	849	C	MET	A	789	33.351	-18.550	18.740	1.00	46.53	C
ATOM	850	O	MET	A	789	32.298	-18.332	19.339	1.00	46.30	O
ATOM	851	CB	MET	A	789	32.078	-17.904	16.692	1.00	42.88	C
ATOM	852	CG	MET	A	789	31.652	-18.055	15.289	1.00	40.10	C
ATOM	853	SD	MET	A	789	30.781	-19.639	15.039	1.00	39.94	S
ATOM	854	CE	MET	A	789	31.367	-19.918	13.360	1.00	39.80	C
ATOM	855	N	LYS	A	790	34.377	-19.207	19.276	1.00	46.73	N
ATOM	856	CA	LYS	A	790	34.504	-19.499	20.684	1.00	47.29	C
ATOM	857	C	LYS	A	790	34.298	-18.286	21.617	1.00	47.14	C
ATOM	858	O	LYS	A	790	33.335	-18.086	22.395	1.00	41.14	O
ATOM	864	N	GLU	A	791	35.298	-17.402	21.574	1.00	49.74	N
ATOM	865	CA	GLU	A	791	35.035	-16.079	22.128	1.00	54.17	C
ATOM	866	C	GLU	A	791	33.575	-15.820	21.756	1.00	54.72	C
ATOM	867	O	GLU	A	791	33.412	-15.836	20.533	1.00	56.68	O
ATOM	868	CB	GLU	A	791	35.789	-14.866	21.576	1.00	55.37	C
ATOM	873	N	SER	A	792	32.611	-15.700	22.649	1.00	54.96	N
ATOM	874	CA	SER	A	792	31.320	-15.308	22.081	1.00	56.01	C
ATOM	875	C	SER	A	792	31.319	-13.894	21.525	1.00	55.93	C
ATOM	876	O	SER	A	792	31.534	-13.369	20.441	1.00	56.99	O
ATOM	877	CB	SER	A	792	30.159	-15.339	23.088	1.00	56.88	C
ATOM	878	OG	SER	A	792	28.830	-15.203	22.563	1.00	55.04	O
ATOM	879	N	SER	A	793	30.849	-13.012	22.417	1.00	55.19	N
ATOM	880	CA	SER	A	793	29.880	-12.009	22.117	1.00	53.38	C
ATOM	881	C	SER	A	793	28.777	-12.446	21.163	1.00	52.62	C
ATOM	882	O	SER	A	793	27.588	-12.315	21.403	1.00	53.16	O
ATOM	883	CB	SER	A	793	30.433	-10.763	21.418	1.00	52.86	C
ATOM	884	OG	SER	A	793	29.233	-9.939	21.333	1.00	48.02	O
ATOM	885	N	PHE	A	794	29.027	-12.777	19.967	1.00	51.54	* N
ATOM	886	CA	PHE	A	794	28.850	-13.098	18.626	1.00	50.15	* C
ATOM	887	C	PHE	A	794	28.847	-14.547	18.156	1.00	46.40	* C
ATOM	888	O	PHE	A	794	28.950	-14.930	17.003	1.00	43.36	* O
ATOM	889	CB	PHE	A	794	30.202	-12.464	18.177	1.00	55.51	* C
ATOM	890	CG	PHE	A	794	30.682	-12.526	16.778	1.00	60.02	* C
ATOM	891	CD1	PHE	A	794	30.179	-11.598	15.865	1.00	60.89	* C
ATOM	892	CD2	PHE	A	794	31.632	-13.457	16.364	1.00	60.44	* C
ATOM	893	CE1	PHE	A	794	30.581	-11.610	14.543	1.00	61.67	* C
ATOM	894	CE2	PHE	A	794	32.053	-13.462	15.050	1.00	60.60	* C
ATOM	895	CZ	PHE	A	794	31.524	-12.542	14.163	1.00	61.60	* C
ATOM	896	N	TYR	A	795	28.848	-15.432	19.149	1.00	44.88	N
ATOM	897	CA	TYR	A	795	28.875	-16.844	19.022	1.00	43.20	C

FIG. 7 CONT'D

ATOM	898	C	TYR	A	795	27.435	-16.972	18.554	1.00	44.86	C
ATOM	899	O	TYR	A	795	27.145	-17.208	17.404	1.00	47.65	O
ATOM	900	CB	TYR	A	795	29.153	-17.693	20.263	1.00	41.61	C
ATOM	901	CG	TYR	A	795	28.903	-19.166	19.892	1.00	41.01	C
ATOM	902	CD1	TYR	A	795	29.684	-19.857	18.966	1.00	40.23	C
ATOM	903	CD2	TYR	A	795	27.785	-19.796	20.437	1.00	39.57	C
ATOM	904	CE1	TYR	A	795	29.389	-21.142	18.604	1.00	40.74	C
ATOM	905	CE2	TYR	A	795	27.498	-21.086	20.062	1.00	41.23	C
ATOM	906	CZ	TYR	A	795	28.305	-21.772	19.172	1.00	41.70	C
ATOM	907	OH	TYR	A	795	27.973	-23.079	18.856	1.00	43.68	O
ATOM	908	N	SER	A	796	26.568	-16.581	19.453	1.00	46.16	N
ATOM	909	CA	SER	A	796	25.114	-16.662	19.359	1.00	45.87	C
ATOM	910	C	SER	A	796	24.518	-16.079	18.078	1.00	45.91	C
ATOM	911	O	SER	A	796	23.462	-16.512	17.578	1.00	46.30	O
ATOM	912	CB	SER	A	796	24.570	-15.808	20.515	1.00	47.01	C
ATOM	913	OG	SER	A	796	23.260	-15.990	20.987	1.00	46.17	O
ATOM	914	N	LEU	A	797	25.184	-14.996	17.668	1.00	42.49	N
ATOM	915	CA	LEU	A	797	24.783	-14.333	16.443	1.00	38.63	C
ATOM	916	C	LEU	A	797	25.315	-15.173	15.310	1.00	37.16	C
ATOM	917	O	LEU	A	797	24.452	-15.538	14.532	1.00	38.13	O
ATOM	918	CB	LEU	A	797	25.218	-12.907	16.361	1.00	34.60	C
ATOM	919	CG	LEU	A	797	25.022	-11.934	15.210	1.00	29.75	C
ATOM	920	CD1	LEU	A	797	23.648	-11.320	15.392	1.00	27.52	C
ATOM	921	CD2	LEU	A	797	26.285	-11.094	15.061	1.00	26.19	C
ATOM	922	N	CYS	A	798	26.559	-15.557	15.306	1.00	34.52	N
ATOM	923	CA	CYS	A	798	26.964	-16.459	14.238	1.00	34.07	C
ATOM	924	C	CYS	A	798	26.137	-17.727	14.117	1.00	35.88	C
ATOM	925	O	CYS	A	798	26.043	-18.169	12.984	1.00	36.71	O
ATOM	926	CB	CYS	A	798	28.403	-16.724	14.440	1.00	28.22	C
ATOM	927	SG	CYS	A	798	29.742	-15.765	13.871	1.00	13.63	S
ATOM	928	N	LEU	A	799	25.533	-18.274	15.154	1.00	37.11	N
ATOM	929	CA	LEU	A	799	24.571	-19.351	15.072	1.00	38.16	C
ATOM	930	C	LEU	A	799	23.464	-18.959	14.096	1.00	39.60	C
ATOM	931	O	LEU	A	799	23.199	-19.658	13.127	1.00	40.08	O
ATOM	932	CB	LEU	A	799	23.863	-19.853	16.341	1.00	36.55	C
ATOM	933	CG	LEU	A	799	24.575	-20.812	17.334	1.00	34.57	C
ATOM	934	CD1	LEU	A	799	23.756	-22.092	17.539	1.00	32.24	C
ATOM	935	CD2	LEU	A	799	26.004	-21.208	17.024	1.00	32.21	C
ATOM	936	N	THR	A	800	22.923	-17.788	14.388	1.00	39.86	N
ATOM	937	CA	THR	A	800	21.807	-17.262	13.604	1.00	38.50	C
ATOM	938	C	THR	A	800	22.049	-16.884	12.168	1.00	35.85	C
ATOM	939	O	THR	A	800	21.247	-17.189	11.308	1.00	33.27	O
ATOM	940	CB	THR	A	800	21.130	-16.234	14.526	1.00	38.27	C
ATOM	941	OG1	THR	A	800	20.410	-17.184	15.375	1.00	37.88	O
ATOM	942	CG2	THR	A	800	20.141	-15.313	13.855	1.00	39.63	C
ATOM	943	N	MET	A	801	23.123	-16.276	11.758	1.00	32.23	N
ATOM	944	CA	MET	A	801	23.652	-16.202	10.437	1.00	30.69	C
ATOM	945	C	MET	A	801	23.697	-17.600	9.852	1.00	34.69	C
ATOM	946	O	MET	A	801	23.156	-17.925	8.797	1.00	32.65	O
ATOM	947	CB	MET	A	801	24.973	-15.439	10.361	1.00	25.50	C
ATOM	948	CG	MET	A	801	24.937	-13.874	10.371	1.00	20.19	C
ATOM	949	SD	MET	A	801	26.590	-13.125	10.114	1.00	12.86	S
ATOM	950	CE	MET	A	801	27.491	-13.695	11.483	1.00	11.55	C
ATOM	951	N	TRP	A	802	24.294	-18.629	10.495	1.00	40.03	N
ATOM	952	CA	TRP	A	802	24.340	-19.972	10.046	1.00	40.74	C
ATOM	953	C	TRP	A	802	23.060	-20.687	9.610	1.00	43.79	C
ATOM	954	O	TRP	A	802	23.007	-21.746	8.944	1.00	42.65	O
ATOM	955	CB	TRP	A	802	24.731	-20.795	11.251	1.00	37.09	C
ATOM	956	CG	TRP	A	802	25.729	-21.736	10.655	1.00	37.79	C
ATOM	957	CD1	TRP	A	802	25.698	-22.406	9.492	1.00	37.41	C
ATOM	958	CD2	TRP	A	802	26.988	-22.048	11.248	1.00	38.74	C
ATOM	959	NE1	TRP	A	802	26.832	-23.097	9.345	1.00	38.42	N
ATOM	960	CE2	TRP	A	802	27.657	-22.896	10.390	1.00	38.04	C
ATOM	961	CE3	TRP	A	802	27.571	-21.672	12.483	1.00	39.53	C

FIG. 7 CONT'D

ATOM	962	CZ2	TRP	A	802	28.884	-23.425	10.689	1.00	40.55	C
ATOM	963	CZ3	TRP	A	802	28.798	-22.122	12.816	1.00	40.22	C
ATOM	964	CH2	TRP	A	802	29.415	-22.988	11.901	1.00	42.93	C
ATOM	965	N	GLN	A	803	21.885	-20.148	9.969	1.00	44.65	N
ATOM	966	CA	GLN	A	803	20.602	-20.724	9.595	1.00	43.35	C
ATOM	967	C	GLN	A	803	20.361	-20.712	8.075	1.00	41.04	C
ATOM	968	O	GLN	A	803	19.619	-21.522	7.519	1.00	39.10	O
ATOM	969	CB	GLN	A	803	19.526	-19.915	10.296	1.00	42.19	C
ATOM	970	CG	GLN	A	803	19.335	-19.977	11.747	1.00	43.83	C
ATOM	971	CD	GLN	A	803	18.095	-19.289	12.242	1.00	47.78	C
ATOM	972	OE1	GLN	A	803	17.974	-18.095	12.592	1.00	49.72	O
ATOM	973	NE2	GLN	A	803	17.048	-20.114	12.305	1.00	49.90	N
ATOM	974	N	ILE	A	804	20.887	-19.701	7.404	1.00	37.94	N
ATOM	975	CA	ILE	A	804	20.618	-19.418	6.048	1.00	33.28	C
ATOM	976	C	ILE	A	804	21.310	-20.450	5.192	1.00	30.18	C
ATOM	977	O	ILE	A	804	20.526	-21.004	4.435	1.00	27.93	O
ATOM	978	CB	ILE	A	804	20.836	-18.043	5.434	1.00	33.90	C
ATOM	979	CG1	ILE	A	804	20.180	-16.775	5.971	1.00	31.36	C
ATOM	980	CG2	ILE	A	804	20.371	-18.086	3.936	1.00	35.06	C
ATOM	981	CD1	ILE	A	804	20.634	-15.509	5.172	1.00	29.14	C
ATOM	982	N	PRO	A	805	22.579	-20.732	5.316	1.00	28.03	N
ATOM	983	CA	PRO	A	805	23.243	-21.717	4.471	1.00	28.64	C
ATOM	984	C	PRO	A	805	22.722	-23.079	4.811	1.00	31.07	C
ATOM	985	O	PRO	A	805	22.759	-23.862	3.935	1.00	32.44	O
ATOM	986	CB	PRO	A	805	24.732	-21.567	4.605	1.00	25.50	C
ATOM	987	CG	PRO	A	805	24.926	-20.752	5.823	1.00	25.19	C
ATOM	988	CD	PRO	A	805	23.604	-20.038	6.096	1.00	29.00	C
ATOM	989	N	GLN	A	806	22.155	-23.405	5.923	1.00	34.19	N
ATOM	990	CA	GLN	A	806	21.508	-24.609	6.270	1.00	36.51	C
ATOM	991	C	GLN	A	806	20.265	-24.794	5.447	1.00	38.90	C
ATOM	992	O	GLN	A	806	20.042	-25.859	4.863	1.00	42.05	O
ATOM	993	CB	GLN	A	806	21.091	-24.810	7.715	1.00	37.41	C
ATOM	994	CG	GLN	A	806	22.255	-24.819	8.723	1.00	39.98	C
ATOM	995	CD	GLN	A	806	23.391	-25.699	8.220	1.00	42.48	C
ATOM	996	OE1	GLN	A	806	23.808	-25.686	7.038	1.00	40.81	O
ATOM	997	NE2	GLN	A	806	23.932	-26.569	9.131	1.00	45.81	N
ATOM	998	N	GLU	A	807	19.514	-23.702	5.307	1.00	38.88	N
ATOM	999	CA	GLU	A	807	18.220	-23.768	4.635	1.00	35.01	C
ATOM	1000	C	GLU	A	807	18.428	-23.922	3.152	1.00	32.34	C
ATOM	1001	O	GLU	A	807	17.528	-24.422	2.496	1.00	28.93	O
ATOM	1002	CB	GLU	A	807	17.338	-22.613	5.053	1.00	33.00	C
ATOM	1003	CG	GLU	A	807	15.812	-22.802	4.882	1.00	34.10	C
ATOM	1004	CD	GLU	A	807	15.330	-24.158	5.402	1.00	35.77	C
ATOM	1005	OE1	GLU	A	807	15.977	-24.535	6.415	1.00	33.38	OE2 O
ATOM	1006	OE2	GLU	A	807	14.401	-24.879	4.873	1.00	33.87	OE1 O
ATOM	1007	N	PHE	A	808	19.539	-23.528	2.615	1.00	32.52	N
ATOM	1008	CA	PHE	A	808	19.945	-23.545	1.244	1.00	33.74	C
ATOM	1009	C	PHE	A	808	20.403	-24.941	0.809	1.00	35.62	C
ATOM	1010	O	PHE	A	808	20.127	-25.395	-0.276	1.00	35.37	O
ATOM	1011	CB	PHE	A	808	21.054	-22.565	0.914	1.00	27.94	C
ATOM	1012	CG	PHE	A	808	20.750	-21.143	0.640	1.00	23.58	C
ATOM	1013	CD1	PHE	A	808	19.507	-20.596	0.852	1.00	24.07	C
ATOM	1014	CD2	PHE	A	808	21.747	-20.289	0.180	1.00	20.30	C
ATOM	1015	CE1	PHE	A	808	19.305	-19.234	0.586	1.00	24.21	C
ATOM	1016	CE2	PHE	A	808	21.617	-18.968	-0.072	1.00	17.63	C
ATOM	1017	CZ	PHE	A	808	20.354	-18.467	0.114	1.00	21.26	C
ATOM	1018	N	VAL	A	809	21.149	-25.593	1.661	1.00	37.02	N
ATOM	1019	CA	VAL	A	809	21.574	-26.966	1.686	1.00	35.82	C
ATOM	1020	C	VAL	A	809	20.303	-27.762	1.774	1.00	36.82	C
ATOM	1021	O	VAL	A	809	20.074	-28.669	0.981	1.00	36.45	O
ATOM	1022	CB	VAL	A	809	22.485	-27.170	2.902	1.00	33.36	C
ATOM	1023	CG1	VAL	A	809	22.457	-28.467	3.646	1.00	30.83	C
ATOM	1024	CG2	VAL	A	809	23.963	-26.983	2.507	1.00	30.59	C
ATOM	1025	N	LYS	A	810	19.458	-27.378	2.717	1.00	39.04	N

FIG. 7 CONT'D

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ATOM   1026  CA  LYS A 810      18.196 -28.092   2.882  1.00 41.60           C
ATOM   1027  C   LYS A 810      17.444 -27.951   1.590  1.00 44.27           C
ATOM   1028  O   LYS A 810      17.050 -28.994   1.058  1.00 46.87           O
ATOM   1029  CB  LYS A 810      17.368 -27.715   4.070  1.00 40.46           C
ATOM   1030  CG  LYS A 810      16.003 -28.233   4.434  1.00 39.57           C
ATOM   1031  CD  LYS A 810      15.605 -28.321   5.898  1.00 37.60           C
ATOM   1032  CE  LYS A 810      16.227 -27.541   7.006  1.00 36.30           C
ATOM   1033  NZ  LYS A 810      15.467 -26.591   7.844  1.00 33.01           N
ATOM   1034  N   LEU A 811      17.316 -26.743   1.015  1.00 45.15           N
ATOM   1035  CA  LEU A 811      16.382 -26.613  -0.106  1.00 43.08           C
ATOM   1036  C   LEU A 811      17.008 -26.956  -1.444  1.00 41.94           C
ATOM   1037  O   LEU A 811      16.346 -27.012  -2.477  1.00 39.52           O
ATOM   1038  CB  LEU A 811      15.711 -25.226  -0.070  1.00 40.28           C
ATOM   1039  CG  LEU A 811      14.500 -25.101   0.864  1.00 37.82           C
ATOM   1040  CD1 LEU A 811      14.314 -23.719   1.507  1.00 36.40           C
ATOM   1041  CD2 LEU A 811      13.240 -25.529   0.174  1.00 33.74           C
ATOM   1042  N   GLN A 812      18.290 -27.169  -1.489  1.00 42.06           N
ATOM   1043  CA  GLN A 812      19.136 -27.290  -2.648  1.00 43.78           C
ATOM   1044  C   GLN A 812      18.716 -26.202  -3.633  1.00 45.07           C
ATOM   1045  O   GLN A 812      17.973 -26.422  -4.584  1.00 46.82           O
ATOM   1046  CB  GLN A 812      19.240 -28.662  -3.216  1.00 44.72           C
ATOM   1047  CG  GLN A 812      20.137 -29.852  -3.096  1.00 44.12           C
ATOM   1048  CD  GLN A 812      19.726 -31.235  -3.469  1.00 44.16           C
ATOM   1049  OE1 GLN A 812      19.914 -32.299  -2.856  1.00 46.06           O
ATOM   1050  NE2 GLN A 812      19.061 -31.443  -4.590  1.00 45.38           N
ATOM   1051  N   VAL A 813      19.146 -24.969  -3.303  1.00 42.21           N
ATOM   1052  CA  VAL A 813      19.014 -23.730  -4.000  1.00 35.60           C
ATOM   1053  C   VAL A 813      20.051 -23.621  -5.085  1.00 33.67           C
ATOM   1054  O   VAL A 813      21.214 -23.840  -5.031  1.00 29.58           O
ATOM   1055  CB  VAL A 813      18.993 -22.555  -3.003  1.00 34.01           C
ATOM   1056  CG1 VAL A 813      18.923 -21.150  -3.613  1.00 30.54           C
ATOM   1057  CG2 VAL A 813      17.706 -22.753  -2.180  1.00 30.70           C
ATOM   1058  N   SER A 814      19.527 -23.325  -6.247  1.00 32.14           N
ATOM   1059  CA  SER A 814      20.251 -23.161  -7.482  1.00 31.17           C
ATOM   1060  C   SER A 814      20.751 -21.742  -7.644  1.00 32.78           C
ATOM   1061  O   SER A 814      20.215 -20.803  -7.093  1.00 32.55           O
ATOM   1062  CB  SER A 814      19.302 -23.383  -8.669  1.00 24.49           C
ATOM   1063  OG  SER A 814      18.078 -22.776  -8.317  1.00 17.51           O
ATOM   1064  N   GLN A 815      21.733 -21.557  -8.462  1.00 33.63           N
ATOM   1065  CA  GLN A 815      22.159 -20.225  -8.833  1.00 37.49           C
ATOM   1066  C   GLN A 815      21.160 -19.252  -9.398  1.00 39.21           C
ATOM   1067  O   GLN A 815      21.229 -18.059  -9.243  1.00 40.38           O
ATOM   1068  CB  GLN A 815      23.213 -20.514  -9.880  1.00 35.64           C
ATOM   1069  CG  GLN A 815      23.550 -19.282 -10.691  1.00 36.98           C
ATOM   1070  CD  GLN A 815      24.705 -18.820  -9.832  1.00 38.49           C
ATOM   1071  OE1 GLN A 815      24.500 -18.283  -8.750  1.00 41.78           O
ATOM   1072  NE2 GLN A 815      25.831 -19.177 -10.392  1.00 39.43           N
ATOM   1073  N   GLU A 816      20.236 -19.658 -10.226  1.00 38.66           N
ATOM   1074  CA  GLU A 816      19.262 -18.884 -10.900  1.00 36.72           C
ATOM   1075  C   GLU A 816      18.333 -18.529  -9.752  1.00 35.60           C
ATOM   1076  O   GLU A 816      18.018 -17.334  -9.770  1.00 36.96           O
ATOM   1077  CB  GLU A 816      18.625 -19.538 -12.116  1.00 35.85           C
ATOM   1078  CG  GLU A 816      19.490 -20.070 -13.227  1.00 35.75           C
ATOM   1079  CD  GLU A 816      20.519 -21.193 -13.044  1.00 35.16           C
ATOM   1080  OE1 GLU A 816      20.515 -22.294 -12.438  1.00 30.50           O
ATOM   1081  OE2 GLU A 816      21.631 -20.975 -13.654  1.00 35.78           O
ATOM   1082  N   GLU A 817      18.005 -19.376  -8.812  1.00 33.18           N
ATOM   1083  CA  GLU A 817      16.911 -18.982  -7.931  1.00 32.53           C
ATOM   1084  C   GLU A 817      17.497 -17.917  -7.009  1.00 31.97           C
ATOM   1085  O   GLU A 817      16.916 -16.835  -6.966  1.00 34.01           O
ATOM   1086  CB  GLU A 817      16.085 -20.003  -7.240  1.00 30.67           C
ATOM   1087  CG  GLU A 817      15.125 -20.970  -7.847  1.00 28.72           C
ATOM   1088  CD  GLU A 817      15.098 -22.261  -7.006  1.00 31.53           C
ATOM   1089  OE1 GLU A 817      15.747 -22.284  -5.884  1.00 29.79           O
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FIG. 7 CONT'D

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ATOM   1090  OE2 GLU A 817      14.398 -23.273  -7.322  1.00 28.99           O
ATOM   1091  N   PHE A 818      18.640 -18.124  -6.440  1.00 28.34           N
ATOM   1092  CA  PHE A 818      19.482 -17.194  -5.761  1.00 23.19           C
ATOM   1093  C   PHE A 818      19.589 -15.805  -6.424  1.00 20.86           C
ATOM   1094  O   PHE A 818      19.437 -14.811  -5.687  1.00 19.73           O
ATOM   1095  CB  PHE A 818      20.909 -17.822  -5.630  1.00 20.95           C
ATOM   1096  CG  PHE A 818      21.851 -16.864  -4.961  1.00 23.47           C
ATOM   1097  CD1 PHE A 818      21.645 -16.494  -3.603  1.00 23.27           C
ATOM   1098  CD2 PHE A 818      22.928 -16.304  -5.661  1.00 21.87           C
ATOM   1099  CE1 PHE A 818      22.503 -15.622  -2.969  1.00 21.17           C
ATOM   1100  CE2 PHE A 818      23.765 -15.447  -5.016  1.00 20.87           C
ATOM   1101  CZ  PHE A 818      23.564 -15.121  -3.672  1.00 21.44           C
ATOM   1102  N   LEU A 819      19.899 -15.711  -7.716  1.00 14.72           N
ATOM   1103  CA  LEU A 819      20.071 -14.445  -8.329  1.00 10.65           C
ATOM   1104  C   LEU A 819      18.796 -13.628  -8.249  1.00  9.47           C
ATOM   1105  O   LEU A 819      18.615 -12.456  -7.883  1.00  7.78           O
ATOM   1106  CB  LEU A 819      20.753 -14.632  -9.650  1.00  9.15           C
ATOM   1107  CG  LEU A 819      22.152 -15.280  -9.718  1.00  8.54           C
ATOM   1108  CD1 LEU A 819      22.483 -16.050 -11.077  1.00  2.14           C
ATOM   1109  CD2 LEU A 819      23.101 -14.226  -9.227  1.00  2.02           C
ATOM   1110  N   CYS A 820      17.628 -14.187  -8.527  1.00  3.91           N
ATOM   1111  CA  CYS A 820      16.335 -13.692  -8.547  1.00 10.94           C
ATOM   1112  C   CYS A 820      15.906 -13.439  -7.131  1.00 13.15           C
ATOM   1113  O   CYS A 820      15.304 -12.366  -7.070  1.00 11.97           O
ATOM   1114  CB  CYS A 820      15.311 -14.506  -9.375  1.00 10.26           C
ATOM   1115  SG  CYS A 820      15.777 -14.993 -11.027  1.00  5.05           S
ATOM   1116  N   MET A 821      16.201 -14.173  -6.075  1.00 16.16           N
ATOM   1117  CA  MET A 821      15.587 -13.865  -4.793  1.00 14.73           C
ATOM   1118  C   MET A 821      16.416 -12.752  -4.221  1.00 16.24           C
ATOM   1119  O   MET A 821      15.902 -11.924  -3.492  1.00 17.00           O
ATOM   1120  CB  MET A 821      15.454 -14.945  -3.768  1.00 13.38           C
ATOM   1121  CG  MET A 821      15.584 -16.318  -4.360  1.00 16.63           C
ATOM   1122  SD  MET A 821      15.517 -17.824  -3.415  1.00 12.19           S
ATOM   1123  CE  MET A 821      14.612 -17.058  -1.989  1.00  7.32           C
ATOM   1124  N   LYS A 822      17.686 -12.726  -4.569  1.00 16.81           N
ATOM   1125  CA  LYS A 822      18.474 -11.620  -3.968  1.00 16.55           C
ATOM   1126  C   LYS A 822      17.888 -10.330  -4.523  1.00 20.30           C
ATOM   1127  O   LYS A 822      17.475  -9.522  -3.653  1.00 21.69           O
ATOM   1128  CB  LYS A 822      19.906 -12.015  -4.099  1.00 10.66           C
ATOM   1129  CG  LYS A 822      20.836 -10.844  -4.361  1.00 10.10           C
ATOM   1130  CD  LYS A 822      22.239 -11.279  -3.963  1.00  9.66           C
ATOM   1131  CE  LYS A 822      23.138 -11.584  -5.135  1.00 10.01           C
ATOM   1132  NZ  LYS A 822      23.392 -10.224  -5.793  1.00 12.25           N
ATOM   1133  N   VAL A 823      17.574 -10.146  -5.863  1.00 18.08           N
ATOM   1134  CA  VAL A 823      16.985  -8.900  -6.325  1.00 12.47           C
ATOM   1135  C   VAL A 823      15.739  -8.661  -5.520  1.00 13.11           C
ATOM   1136  O   VAL A 823      15.459  -7.541  -5.258  1.00 14.54           O
ATOM   1137  CB  VAL A 823      16.443  -8.823  -7.759  1.00  3.39           C
ATOM   1138  CG1 VAL A 823      15.740  -7.514  -8.068  1.00  2.96           C
ATOM   1139  CG2 VAL A 823      17.491  -9.054  -8.839  1.00  5.71           C
ATOM   1140  N   LEU A 824      14.962  -9.667  -5.264  1.00 13.59           N
ATOM   1141  CA  LEU A 824      13.799  -9.555  -4.440  1.00 15.00           C
ATOM   1142  C   LEU A 824      14.138  -8.937  -3.125  1.00 17.88           C
ATOM   1143  O   LEU A 824      13.222  -8.206  -2.772  1.00 19.65           O
ATOM   1144  CB  LEU A 824      12.959 -10.860  -4.336  1.00 13.78           C
ATOM   1145  CG  LEU A 824      12.287 -11.192  -5.722  1.00 10.74           C
ATOM   1146  CD1 LEU A 824      11.469 -12.439  -5.612  1.00  9.44           C
ATOM   1147  CD2 LEU A 824      11.565  -9.976  -6.301  1.00  7.32           C
ATOM   1148  N   LEU A 825      15.260  -9.144  -2.429  1.00 19.40           N
ATOM   1149  CA  LEU A 825      15.448  -8.561  -1.114  1.00 17.82           C
ATOM   1150  C   LEU A 825      15.872  -7.103  -1.182  1.00 17.25           C
ATOM   1151  O   LEU A 825      16.005  -6.390  -0.160  1.00 17.96           O
ATOM   1152  CB  LEU A 825      16.608  -9.218  -0.364  1.00 15.99           C
ATOM   1153  CG  LEU A 825      16.409 -10.597   0.249  1.00 14.49           C
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FIG. 7 CONT'D

ATOM	1154	CD1	LEU	A	825	17.876	-11.067	0.411	1.00	12.08	C
ATOM	1155	CD2	LEU	A	825	15.494	-10.443	1.438	1.00	10.65	C
ATOM	1156	N	LEU	A	826	16.332	-6.692	-2.357	1.00	14.74	N
ATOM	1157	CA	LEU	A	826	16.733	-5.364	-2.650	1.00	11.11	C
ATOM	1158	C	LEU	A	826	15.411	-4.575	-2.760	1.00	14.46	C
ATOM	1159	O	LEU	A	826	15.370	-3.385	-2.307	1.00	14.92	O
ATOM	1160	CB	LEU	A	826	17.533	-5.280	-3.898	1.00	5.38	C
ATOM	1161	CG	LEU	A	826	17.825	-3.907	-4.489	1.00	3.89	C
ATOM	1162	CD1	LEU	A	826	18.038	-2.919	-3.282	1.00	3.95	C
ATOM	1163	CD2	LEU	A	826	18.986	-3.598	-5.441	1.00	5.93	C
ATOM	1164	N	LEU	A	827	14.391	-5.306	-3.286	1.00	10.64	N
ATOM	1165	CA	LEU	A	827	13.089	-4.741	-3.285	1.00	10.64	C
ATOM	1166	C	LEU	A	827	12.213	-5.204	-2.164	1.00	15.58	C
ATOM	1167	O	LEU	A	827	11.001	-5.159	-2.408	1.00	16.53	O
ATOM	1168	CB	LEU	A	827	12.423	-4.981	-4.676	1.00	6.75	C
ATOM	1169	CG	LEU	A	827	13.407	-4.837	-5.878	1.00	2.05	C
ATOM	1170	CD1	LEU	A	827	12.520	-5.230	-7.103	1.00	2.73	C
ATOM	1171	CD2	LEU	A	827	14.050	-3.482	-5.931	1.00	3.01	C
ATOM	1172	N	ASN	A	828	12.667	-5.642	-1.018	1.00	17.78	N
ATOM	1173	CA	ASN	A	828	11.874	-6.143	0.050	1.00	22.44	C
ATOM	1174	C	ASN	A	828	11.192	-5.284	1.053	1.00	23.72	C
ATOM	1175	O	ASN	A	828	10.225	-5.776	1.620	1.00	23.24	O
ATOM	1176	CB	ASN	A	828	12.629	-7.199	0.891	1.00	23.66	C
ATOM	1177	CG	ASN	A	828	11.968	-8.570	0.801	1.00	22.87	C
ATOM	1178	OD1	ASN	A	828	10.806	-8.801	0.544	1.00	21.94	O
ATOM	1179	ND2	ASN	A	828	12.666	-9.670	1.029	1.00	22.59	N
ATOM	1180	N	THR	A	829	11.575	-4.097	1.360	1.00	25.98	N
ATOM	1181	CA	THR	A	829	11.119	-3.210	2.437	1.00	28.91	C
ATOM	1182	C	THR	A	829	10.937	-1.797	1.903	1.00	30.23	C
ATOM	1183	O	THR	A	829	11.980	-1.401	1.368	1.00	31.01	O
ATOM	1184	CB	THR	A	829	12.362	-3.092	3.385	1.00	27.58	C
ATOM	1185	OG1	THR	A	829	12.810	-4.409	3.609	1.00	24.71	O
ATOM	1186	CG2	THR	A	829	12.241	-2.254	4.609	1.00	25.74	C
ATOM	1187	N	ILE	A	830	9.828	-1.099	2.034	1.00	32.01	N
ATOM	1188	CA	ILE	A	830	9.827	0.336	1.698	1.00	34.45	C
ATOM	1189	C	ILE	A	830	9.432	1.203	2.883	1.00	35.20	C
ATOM	1190	O	ILE	A	830	8.817	0.626	3.757	1.00	35.55	O
ATOM	1191	CB	ILE	A	830	8.838	0.649	0.530	1.00	33.27	C
ATOM	1192	CG1	ILE	A	830	7.411	0.348	1.010	1.00	30.24	C
ATOM	1193	CG2	ILE	A	830	9.244	-0.052	-0.767	1.00	33.89	C
ATOM	1194	CD1	ILE	A	830	6.357	0.331	-0.038	1.00	27.77	C
ATOM	1195	N	PRO	A	831	9.640	2.511	2.829	1.00	36.30	N
ATOM	1196	CA	PRO	A	831	9.021	3.444	3.762	1.00	37.97	C
ATOM	1197	C	PRO	A	831	7.552	3.222	4.033	1.00	40.63	C
ATOM	1198	O	PRO	A	831	6.798	2.829	3.154	1.00	41.54	O
ATOM	1199	CB	PRO	A	831	9.205	4.784	3.101	1.00	34.04	C
ATOM	1200	CG	PRO	A	831	10.162	4.642	2.004	1.00	33.59	C
ATOM	1201	CD	PRO	A	831	10.280	3.191	1.680	1.00	34.17	C
ATOM	1202	N	LEU	A	832	7.062	3.520	5.218	1.00	42.58	N
ATOM	1203	CA	LEU	A	832	5.629	3.557	5.476	1.00	44.66	C
ATOM	1204	C	LEU	A	832	4.787	4.433	4.573	1.00	46.81	C
ATOM	1205	O	LEU	A	832	3.598	4.131	4.356	1.00	47.94	O
ATOM	1206	CB	LEU	A	832	5.514	3.952	6.940	1.00	42.47	C
ATOM	1207	CG	LEU	A	832	5.912	2.994	8.067	1.00	40.16	C
ATOM	1208	CD1	LEU	A	832	6.038	3.766	9.376	1.00	38.05	C
ATOM	1209	CD2	LEU	A	832	4.848	1.938	8.312	1.00	36.99	C
ATOM	1210	N	GLU	A	833	5.311	5.507	3.998	1.00	48.02	N
ATOM	1211	CA	GLU	A	833	4.672	6.426	3.070	1.00	47.17	C
ATOM	1212	C	GLU	A	833	4.945	5.971	1.641	1.00	46.42	C
ATOM	1213	O	GLU	A	833	4.616	6.723	0.732	1.00	48.67	O
ATOM	1214	CB	GLU	A	833	5.052	7.851	3.370	1.00	46.12	C
ATOM	1215	CG	GLU	A	833	6.421	8.455	3.351	1.00	46.42	C
ATOM	1216	CD	GLU	A	833	7.424	7.989	4.385	1.00	47.67	C
ATOM	1217	OE1	GLU	A	833	7.550	6.739	4.455	1.00	47.74	O

FIG. 7 CONT'D

ATOM	1218	OE2	GLU	A	833	8.179	8.685	5.133	1.00	47.00	O
ATOM	1219	N	GLY	A	834	5.481	4.776	1.415	1.00	42.93	N
ATOM	1220	CA	GLY	A	834	6.040	4.269	0.229	1.00	38.78	C
ATOM	1221	C	GLY	A	834	7.121	5.045	-0.454	1.00	39.18	C
ATOM	1222	O	GLY	A	834	7.668	6.010	0.047	1.00	38.48	O
ATOM	1223	N	LEU	A	835	7.453	4.709	-1.693	1.00	39.67	N
ATOM	1224	CA	LEU	A	835	8.505	5.301	-2.505	1.00	38.03	C
ATOM	1225	C	LEU	A	835	8.047	6.519	-3.282	1.00	37.62	C
ATOM	1226	O	LEU	A	835	6.873	6.727	-3.385	1.00	37.44	O
ATOM	1227	CB	LEU	A	835	9.072	4.238	-3.470	1.00	35.40	C
ATOM	1228	CG	LEU	A	835	9.747	2.994	-2.882	1.00	33.33	C
ATOM	1229	CD1	LEU	A	835	10.056	1.914	-3.886	1.00	31.00	C
ATOM	1230	CD2	LEU	A	835	11.091	3.364	-2.246	1.00	32.85	C
ATOM	1231	N	ARG	A	836	8.969	7.313	-3.792	1.00	39.11	N
ATOM	1232	CA	ARG	A	836	8.667	8.280	-4.829	1.00	39.86	C
ATOM	1233	C	ARG	A	836	8.255	7.561	-6.104	1.00	37.52	C
ATOM	1234	O	ARG	A	836	7.159	7.865	-6.537	1.00	41.35	O
ATOM	1235	CB	ARG	A	836	9.797	9.186	-5.210	1.00	42.59	C
ATOM	1236	CG	ARG	A	836	10.598	9.933	-4.164	1.00	46.05	C
ATOM	1237	CD	ARG	A	836	11.330	11.107	-4.767	1.00	47.02	C
ATOM	1238	NE	ARG	A	836	10.546	12.294	-5.052	1.00	48.85	N
ATOM	1239	CZ	ARG	A	836	9.800	12.747	-6.028	1.00	48.40	C
ATOM	1240	NH1	ARG	A	836	9.671	12.017	-7.141	1.00	49.88	N
ATOM	1241	NH2	ARG	A	836	9.157	13.899	-5.980	1.00	47.83	N
ATOM	1242	N	SER	A	837	8.935	6.628	-6.721	1.00	32.46	N
ATOM	1243	CA	SER	A	837	8.454	5.890	-7.850	1.00	28.24	C
ATOM	1244	C	SER	A	837	7.716	4.591	-7.519	1.00	28.46	C
ATOM	1245	O	SER	A	837	8.058	3.493	-8.045	1.00	24.59	O
ATOM	1246	CB	SER	A	837	9.572	5.451	-8.749	1.00	26.82	C
ATOM	1247	OG	SER	A	837	10.713	6.134	-8.929	1.00	25.09	O
ATOM	1248	N	GLN	A	838	6.726	4.630	-6.629	1.00	28.91	N
ATOM	1249	CA	GLN	A	838	5.948	3.411	-6.395	1.00	30.03	C
ATOM	1250	C	GLN	A	838	5.684	2.597	-7.657	1.00	31.27	C
ATOM	1251	O	GLN	A	838	6.090	1.460	-7.844	1.00	34.74	O
ATOM	1252	CB	GLN	A	838	4.550	3.508	-5.752	1.00	28.30	C
ATOM	1253	CG	GLN	A	838	3.991	2.334	-4.994	1.00	27.09	C
ATOM	1254	CD	GLN	A	838	4.958	1.859	-3.842	1.00	28.19	C
ATOM	1255	OE1	GLN	A	838	4.992	2.520	-2.790	1.00	23.78	O
ATOM	1256	NE2	GLN	A	838	5.745	0.775	-4.040	1.00	26.30	N
ATOM	1257	N	THR	A	839	4.868	3.016	-8.564	1.00	32.56	N
ATOM	1258	CA	THR	A	839	4.521	2.329	-9.790	1.00	32.74	C
ATOM	1259	C	THR	A	839	5.680	1.647	-10.461	1.00	32.54	C
ATOM	1260	O	THR	A	839	5.563	0.424	-10.478	1.00	31.21	O
ATOM	1261	CB	THR	A	839	3.727	3.395	-10.631	1.00	32.90	C
ATOM	1262	OG1	THR	A	839	2.947	4.193	-9.700	1.00	29.91	O
ATOM	1263	CG2	THR	A	839	2.886	2.758	-11.726	1.00	27.75	C
ATOM	1264	N	GLN	A	840	6.727	2.246	-11.001	1.00	32.03	N
ATOM	1265	CA	GLN	A	840	7.931	1.546	-11.461	1.00	32.77	C
ATOM	1266	C	GLN	A	840	8.495	0.495	-10.498	1.00	30.32	C
ATOM	1267	O	GLN	A	840	8.840	-0.624	-10.770	1.00	27.01	O
ATOM	1268	CB	GLN	A	840	9.019	2.588	-11.823	1.00	33.45	C
ATOM	1269	CG	GLN	A	840	8.348	3.917	-11.959	1.00	38.87	C
ATOM	1270	CD	GLN	A	840	8.859	5.307	-12.091	1.00	41.75	C
ATOM	1271	OE1	GLN	A	840	8.579	6.184	-11.258	1.00	42.40	O
ATOM	1272	NE2	GLN	A	840	9.580	5.742	-13.134	1.00	42.45	N
ATOM	1273	N	PHE	A	841	8.664	0.790	-9.205	1.00	27.08	N
ATOM	1274	CA	PHE	A	841	8.865	-0.090	-8.155	1.00	23.85	C
ATOM	1275	C	PHE	A	841	8.004	-1.320	-8.373	1.00	25.77	C
ATOM	1276	O	PHE	A	841	8.500	-2.470	-8.334	1.00	23.68	O
ATOM	1277	CB	PHE	A	841	8.539	0.396	-6.728	1.00	18.78	C
ATOM	1278	CG	PHE	A	841	8.979	-0.630	-5.674	1.00	11.49	C
ATOM	1279	CD1	PHE	A	841	10.288	-1.034	-5.513	1.00	8.12	C
ATOM	1280	CD2	PHE	A	841	8.026	-1.157	-4.847	1.00	7.96	C
ATOM	1281	CE1	PHE	A	841	10.727	-1.897	-4.583	1.00	2.27	C

FIG. 7 CONT'D

ATOM	1282	CE2	PHE	A	841	8.279	-2.055	-3.921	1.00	2.02		C
ATOM	1283	CZ	PHE	A	841	9.639	-2.331	-3.816	1.00	8.18		C
ATOM	1284	N	GLU	A	842	6.713	-1.074	-8.400	1.00	28.90		N
ATOM	1285	CA	GLU	A	842	5.824	-2.277	-8.243	1.00	32.59		C
ATOM	1286	C	GLU	A	842	6.016	-3.118	-9.502	1.00	33.91		C
ATOM	1287	O	GLU	A	842	6.056	-4.348	-9.540	1.00	31.70		O
ATOM	1288	CB	GLU	A	842	4.601	-1.651	-7.803	1.00	31.01		C
ATOM	1289	CG	GLU	A	842	3.312	-1.476	-7.159	1.00	32.51		C
ATOM	1290	CD	GLU	A	842	3.543	-1.493	-5.693	1.00	34.51		C
ATOM	1291	OE1	GLU	A	842	3.899	-2.604	-5.243	1.00	39.04	OE2	O
ATOM	1292	OE2	GLU	A	842	3.473	-0.503	-4.998	1.00	35.27	OE1	O
ATOM	1293	N	GLU	A	843	6.255	-2.480	-10.656	1.00	35.90		N
ATOM	1294	CA	GLU	A	843	6.496	-3.107	-11.937	1.00	35.38		C
ATOM	1295	C	GLU	A	843	7.738	-4.007	-11.843	1.00	32.64		C
ATOM	1296	O	GLU	A	843	7.760	-5.162	-12.308	1.00	30.91		O
ATOM	1297	CB	GLU	A	843	6.652	-2.234	-13.198	1.00	33.69		C
ATOM	1298	CG	GLU	A	843	5.506	-1.258	-13.303	1.00	38.41		C
ATOM	1299	CD	GLU	A	843	5.348	-0.648	-14.707	1.00	40.94		C
ATOM	1300	OE1	GLU	A	843	6.196	-1.197	-15.480	1.00	43.42		O
ATOM	1301	OE2	GLU	A	843	4.495	0.212	-15.006	1.00	37.30		O
ATOM	1302	N	MET	A	844	8.761	-3.411	-11.237	1.00	28.95		N
ATOM	1303	CA	MET	A	844	10.068	-4.043	-11.150	1.00	23.17		C
ATOM	1304	C	MET	A	844	10.005	-5.255	-10.221	1.00	22.36		C
ATOM	1305	O	MET	A	844	10.440	-6.335	-10.522	1.00	16.42		O
ATOM	1306	CB	MET	A	844	11.053	-2.945	-10.771	1.00	17.35		C
ATOM	1307	CG	MET	A	844	12.470	-3.331	-11.191	1.00	12.38		C
ATOM	1308	SD	MET	A	844	13.621	-2.560	-10.054	1.00	8.94		S
ATOM	1309	CE	MET	A	844	14.720	-3.924	-9.766	1.00	7.41		C
ATOM	1310	N	ARG	A	845	9.339	-5.104	-9.084	1.00	24.09		N
ATOM	1311	CA	ARG	A	845	9.067	-6.171	-8.184	1.00	25.20		C
ATOM	1312	C	ARG	A	845	8.369	-7.218	-8.973	1.00	23.92		C
ATOM	1313	O	ARG	A	845	8.895	-8.293	-8.955	1.00	23.06		O
ATOM	1314	CB	ARG	A	845	8.272	-5.922	-6.919	1.00	28.89		C
ATOM	1315	CG	ARG	A	845	8.590	-6.774	-5.673	1.00	32.65		C
ATOM	1316	CD	ARG	A	845	8.099	-6.256	-4.332	1.00	36.04		C
ATOM	1317	NE	ARG	A	845	8.010	-7.164	-3.250	1.00	38.59		N
ATOM	1318	CZ	ARG	A	845	7.293	-8.056	-2.645	1.00	42.31		C
ATOM	1319	NH1	ARG	A	845	6.063	-8.465	-2.975	1.00	43.62		N
ATOM	1320	NH2	ARG	A	845	7.788	-8.704	-1.554	1.00	44.06		N
ATOM	1321	N	SER	A	846	7.200	-6.990	-9.541	1.00	25.21		N
ATOM	1322	CA	SER	A	846	6.549	-8.009	-10.347	1.00	23.12		C
ATOM	1323	C	SER	A	846	7.258	-8.817	-11.404	1.00	24.76		C
ATOM	1324	O	SER	A	846	7.153	-10.008	-11.617	1.00	24.66		O
ATOM	1325	CB	SER	A	846	5.529	-7.255	-11.153	1.00	16.77		C
ATOM	1326	OG	SER	A	846	4.453	-7.904	-10.553	1.00	14.42		O
ATOM	1327	N	SER	A	847	8.024	-8.106	-12.186	1.00	24.79		N
ATOM	1328	CA	SER	A	847	8.865	-8.658	-13.232	1.00	22.64		C
ATOM	1329	C	SER	A	847	10.022	-9.450	-12.698	1.00	22.51		C
ATOM	1330	O	SER	A	847	10.416	-10.343	-13.457	1.00	25.57		O
ATOM	1331	CB	SER	A	847	9.161	-7.505	-14.206	1.00	19.32		C
ATOM	1332	OG	SER	A	847	10.386	-7.395	-14.860	1.00	12.77		O
ATOM	1333	N	TYR	A	848	10.587	-9.206	-11.536	1.00	20.51		N
ATOM	1334	CA	TYR	A	848	11.360	-10.211	-10.841	1.00	20.11		C
ATOM	1335	C	TYR	A	848	10.636	-11.217	-9.955	1.00	19.44		C
ATOM	1336	O	TYR	A	848	11.178	-12.269	-9.946	1.00	17.19		O
ATOM	1337	CB	TYR	A	848	12.420	-9.613	-9.983	1.00	16.19		C
ATOM	1338	CG	TYR	A	848	13.435	-8.832	-10.769	1.00	11.96		C
ATOM	1339	CD1	TYR	A	848	14.536	-9.497	-11.304	1.00	8.90		C
ATOM	1340	CD2	TYR	A	848	13.346	-7.457	-10.890	1.00	8.58		C
ATOM	1341	CE1	TYR	A	848	15.495	-8.763	-11.932	1.00	2.91		C
ATOM	1342	CE2	TYR	A	848	14.214	-6.737	-11.677	1.00	2.02		C
ATOM	1343	CZ	TYR	A	848	15.328	-7.374	-12.106	1.00	7.26		C
ATOM	1344	OH	TYR	A	848	16.255	-6.652	-12.831	1.00	8.57		O
ATOM	1345	N	ILE	A	849	9.546	-11.137	-9.305	1.00	19.88		N

FIG. 7 CONT'D

ATOM	1346	CA	ILE	A	849	8.812	-12.265	-8.850	1.00	22.48	C
ATOM	1347	C	ILE	A	849	8.678	-13.316	-9.930	1.00	27.06	C
ATOM	1348	O	ILE	A	849	8.994	-14.500	-9.746	1.00	26.00	O
ATOM	1349	CB	ILE	A	849	7.499	-11.764	-8.273	1.00	20.46	C
ATOM	1350	CG1	ILE	A	849	7.734	-11.283	-6.815	1.00	21.79	C
ATOM	1351	CG2	ILE	A	849	6.390	-12.766	-8.264	1.00	17.34	C
ATOM	1352	CD1	ILE	A	849	6.467	-10.750	-6.148	1.00	20.06	C
ATOM	1353	N	ARG	A	850	8.196	-13.030	-11.134	1.00	30.59	N
ATOM	1354	CA	ARG	A	850	8.041	-13.778	-12.338	1.00	28.57	C
ATOM	1355	C	ARG	A	850	9.381	-14.274	-12.903	1.00	29.50	C
ATOM	1356	O	ARG	A	850	9.361	-15.261	-13.666	1.00	29.25	O
ATOM	1357	CB	ARG	A	850	7.423	-12.964	-13.480	1.00	26.92	C
ATOM	1358	CG	ARG	A	850	6.021	-12.617	-13.765	1.00	24.72	C
ATOM	1359	CD	ARG	A	850	5.607	-12.002	-15.065	1.00	19.61	C
ATOM	1360	NE	ARG	A	850	6.134	-10.701	-15.344	1.00	17.31	N
ATOM	1361	CZ	ARG	A	850	5.835	-9.439	-14.996	1.00	13.48	C
ATOM	1362	NH1	ARG	A	850	4.831	-9.058	-14.204	1.00	8.98	N
ATOM	1363	NH2	ARG	A	850	6.665	-8.522	-15.538	1.00	9.34	N
ATOM	1364	N	GLU	A	851	10.511	-13.639	-12.634	1.00	26.73	N
ATOM	1365	CA	GLU	A	851	11.770	-14.220	-13.083	1.00	24.76	C
ATOM	1366	C	GLU	A	851	12.163	-15.471	-12.280	1.00	24.94	C
ATOM	1367	O	GLU	A	851	12.799	-16.399	-12.757	1.00	23.95	O
ATOM	1368	CB	GLU	A	851	12.922	-13.240	-13.172	1.00	20.05	C
ATOM	1369	CG	GLU	A	851	14.086	-13.476	-14.093	1.00	17.87	C
ATOM	1370	CD	GLU	A	851	13.672	-13.852	-15.488	1.00	18.75	C
ATOM	1371	OE1	GLU	A	851	12.702	-14.611	-15.579	1.00	19.21	O
ATOM	1372	OE2	GLU	A	851	14.099	-13.501	-16.587	1.00	17.93	O
ATOM	1373	N	LEU	A	852	11.808	-15.498	-11.005	1.00	25.93	N
ATOM	1374	CA	LEU	A	852	11.958	-16.496	-9.969	1.00	22.56	C
ATOM	1375	C	LEU	A	852	11.076	-17.679	-10.366	1.00	24.62	C
ATOM	1376	O	LEU	A	852	11.607	-18.744	-10.403	1.00	22.02	O
ATOM	1377	CB	LEU	A	852	11.621	-15.994	-8.562	1.00	12.35	C
ATOM	1378	CG	LEU	A	852	11.589	-16.893	-7.305	1.00	2.12	C
ATOM	1379	CD1	LEU	A	852	12.860	-17.609	-7.183	1.00	2.09	C
ATOM	1380	CD2	LEU	A	852	11.048	-16.158	-6.041	1.00	2.58	C
ATOM	1381	N	ILE	A	853	9.814	-17.533	-10.766	1.00	26.55	N
ATOM	1382	CA	ILE	A	853	8.948	-18.527	-11.302	1.00	26.11	C
ATOM	1383	C	ILE	A	853	9.579	-19.067	-12.588	1.00	30.26	C
ATOM	1384	O	ILE	A	853	9.685	-20.318	-12.688	1.00	32.18	O
ATOM	1385	CB	ILE	A	853	7.507	-18.122	-11.489	1.00	21.10	C
ATOM	1386	CG1	ILE	A	853	6.711	-17.833	-10.219	1.00	19.54	C
ATOM	1387	CG2	ILE	A	853	6.721	-19.129	-12.332	1.00	15.80	C
ATOM	1388	CD1	ILE	A	853	5.579	-16.778	-10.235	1.00	15.57	C
ATOM	1389	N	LYS	A	854	10.159	-18.277	-13.467	1.00	31.94	N
ATOM	1390	CA	LYS	A	854	11.121	-18.839	-14.407	1.00	34.31	C
ATOM	1391	C	LYS	A	854	12.209	-19.808	-13.931	1.00	37.21	C
ATOM	1392	O	LYS	A	854	12.587	-20.856	-14.523	1.00	36.51	O
ATOM	1393	CB	LYS	A	854	11.710	-17.757	-15.329	1.00	29.98	C
ATOM	1394	CG	LYS	A	854	11.097	-17.842	-16.723	1.00	29.11	C
ATOM	1395	CD	LYS	A	854	10.539	-16.499	-17.149	1.00	29.22	C
ATOM	1396	CE	LYS	A	854	11.292	-15.920	-18.354	1.00	27.09	C
ATOM	1397	NZ	LYS	A	854	11.140	-14.436	-18.368	1.00	25.56	N
ATOM	1398	N	ALA	A	855	12.933	-19.476	-12.864	1.00	37.86	N
ATOM	1399	CA	ALA	A	855	14.130	-20.210	-12.490	1.00	36.00	C
ATOM	1400	C	ALA	A	855	13.653	-21.496	-11.844	1.00	35.29	C
ATOM	1401	O	ALA	A	855	14.228	-22.525	-12.002	1.00	34.05	O
ATOM	1402	CB	ALA	A	855	14.963	-19.402	-11.531	1.00	31.92	C
ATOM	1403	N	ILE	A	856	12.597	-21.386	-11.066	1.00	35.90	N
ATOM	1404	CA	ILE	A	856	11.939	-22.389	-10.288	1.00	35.30	C
ATOM	1405	C	ILE	A	856	11.560	-23.415	-11.348	1.00	37.00	C
ATOM	1406	O	ILE	A	856	11.942	-24.528	-11.181	1.00	33.52	O
ATOM	1407	CB	ILE	A	856	10.642	-21.978	-9.561	1.00	33.43	C
ATOM	1408	CG1	ILE	A	856	10.758	-20.903	-8.517	1.00	30.66	C
ATOM	1409	CG2	ILE	A	856	9.962	-23.274	-9.035	1.00	33.40	C

FIG. 7 CONT'D

ATOM	1410	CD1	ILE	A	856	9.752	-20.416	-7.509	1.00	27.36	C
ATOM	1411	N	GLY	A	857	10.837	-22.922	-12.369	1.00	39.72	N
ATOM	1412	CA	GLY	A	857	10.735	-23.627	-13.590	1.00	40.91	C
ATOM	1413	C	GLY	A	857	11.801	-24.368	-14.304	1.00	42.29	C
ATOM	1414	O	GLY	A	857	11.538	-25.240	-15.111	1.00	40.99	O
ATOM	1415	N	LEU	A	858	13.075	-24.179	-14.149	1.00	45.58	N
ATOM	1416	CA	LEU	A	858	14.146	-24.709	-14.956	1.00	50.06	C
ATOM	1417	C	LEU	A	858	14.428	-26.142	-14.491	1.00	55.90	C
ATOM	1418	O	LEU	A	858	15.187	-26.832	-15.130	1.00	54.73	O
ATOM	1419	CB	LEU	A	858	15.456	-23.941	-14.974	1.00	44.80	C
ATOM	1420	CG	LEU	A	858	15.739	-22.590	-15.532	1.00	41.49	C
ATOM	1421	CD1	LEU	A	858	16.890	-21.930	-14.810	1.00	40.99	C
ATOM	1422	CD2	LEU	A	858	16.234	-22.672	-16.955	1.00	40.30	C
ATOM	1423	N	ARG	A	859	13.887	-26.519	-13.357	1.00	62.77	N
ATOM	1424	CA	ARG	A	859	14.094	-27.743	-12.656	1.00	70.18	C
ATOM	1425	C	ARG	A	859	12.807	-28.260	-12.041	1.00	73.97	C
ATOM	1426	O	ARG	A	859	12.444	-29.416	-12.271	1.00	75.00	O
ATOM	1427	CB	ARG	A	859	15.216	-27.605	-11.624	1.00	71.50	C
ATOM	1428	CG	ARG	A	859	16.550	-27.954	-12.276	1.00	74.75	C
ATOM	1429	CD	ARG	A	859	17.721	-27.720	-11.348	1.00	77.47	C
ATOM	1430	NE	ARG	A	859	18.908	-27.281	-12.090	1.00	80.36	N
ATOM	1431	CZ	ARG	A	859	19.834	-26.659	-11.355	1.00	83.74	C
ATOM	1432	NH1	ARG	A	859	19.611	-26.495	-10.043	1.00	84.55	N
ATOM	1433	NH2	ARG	A	859	20.931	-26.243	-11.976	1.00	85.61	N
ATOM	1434	N	GLN	A	860	12.057	-27.490	-11.257	1.00	77.89	N
ATOM	1435	CA	GLN	A	860	10.814	-27.992	-10.706	1.00	80.35	C
ATOM	1436	C	GLN	A	860	9.803	-27.850	-11.853	1.00	82.80	C
ATOM	1437	O	GLN	A	860	9.011	-26.932	-11.918	1.00	82.77	O
ATOM	1438	CB	GLN	A	860	10.228	-27.440	-9.448	1.00	79.56	C
ATOM	1439	CG	GLN	A	860	10.922	-27.328	-8.144	1.00	80.20	C
ATOM	1440	CD	GLN	A	860	11.742	-28.430	-7.541	1.00	80.88	C
ATOM	1441	OE1	GLN	A	860	11.903	-28.616	-6.319	1.00	79.65	O
ATOM	1442	NE2	GLN	A	860	12.346	-29.219	-8.441	1.00	81.41	N
ATOM	1443	N	LYS	A	861	9.833	-28.875	-12.696	1.00	85.21	N
ATOM	1444	CA	LYS	A	861	8.760	-29.271	-13.582	1.00	85.60	C
ATOM	1445	C	LYS	A	861	7.751	-30.086	-12.789	1.00	85.35	C
ATOM	1446	O	LYS	A	861	7.733	-31.295	-12.797	1.00	86.47	O
ATOM	1447	CB	LYS	A	861	9.344	-30.038	-14.767	1.00	84.60	C
ATOM	1448	CG	LYS	A	861	10.295	-31.114	-14.298	1.00	84.52	C
ATOM	1449	CD	LYS	A	861	10.846	-32.050	-15.324	1.00	84.98	C
ATOM	1450	CE	LYS	A	861	12.231	-31.688	-15.797	1.00	86.15	C
ATOM	1451	NZ	LYS	A	861	13.341	-31.835	-14.825	1.00	86.38	N
ATOM	1452	N	GLY	A	862	6.936	-29.429	-11.991	1.00	85.45	N
ATOM	1453	CA	GLY	A	862	5.568	-29.827	-11.701	1.00	85.32	C
ATOM	1454	C	GLY	A	862	4.668	-28.688	-12.206	1.00	84.72	C
ATOM	1455	O	GLY	A	862	4.816	-28.032	-13.240	1.00	84.32	O
ATOM	1456	N	VAL	A	863	3.622	-28.462	-11.429	1.00	84.39	N
ATOM	1457	CA	VAL	A	863	2.687	-27.350	-11.429	1.00	83.02	C
ATOM	1458	C	VAL	A	863	2.130	-27.300	-9.994	1.00	82.35	C
ATOM	1459	O	VAL	A	863	1.791	-26.290	-9.405	1.00	83.48	O
ATOM	1460	CB	VAL	A	863	1.615	-27.394	-12.505	1.00	82.29	C
ATOM	1461	CG1	VAL	A	863	1.300	-28.816	-12.983	1.00	81.89	C
ATOM	1462	CG2	VAL	A	863	0.308	-26.718	-12.085	1.00	81.91	C
ATOM	1463	N	VAL	A	864	2.121	-28.492	-9.429	1.00	80.00	N
ATOM	1464	CA	VAL	A	864	2.073	-28.773	-8.002	1.00	76.87	C
ATOM	1465	C	VAL	A	864	3.405	-28.460	-7.337	1.00	74.94	C
ATOM	1466	O	VAL	A	864	3.376	-27.611	-6.448	1.00	74.39	O
ATOM	1467	CB	VAL	A	864	1.635	-30.251	-7.992	1.00	75.56	C
ATOM	1468	CG1	VAL	A	864	2.378	-31.077	-6.952	1.00	76.73	C
ATOM	1469	CG2	VAL	A	864	0.137	-30.296	-7.808	1.00	74.32	C
ATOM	1470	N	SER	A	865	4.497	-29.092	-7.778	1.00	72.58	N
ATOM	1471	CA	SER	A	865	5.800	-28.908	-7.155	1.00	70.35	C
ATOM	1472	C	SER	A	865	6.316	-27.479	-7.321	1.00	67.66	C
ATOM	1473	O	SER	A	865	6.500	-26.734	-6.351	1.00	67.17	O

FIG. 7 CONT'D

ATOM	1474	CB	SER	A	865	6.847	-29.925	-7.620	1.00	71.19	C
ATOM	1475	OG	SER	A	865	7.822	-30.104	-6.581	1.00	72.04	O
ATOM	1476	N	SER	A	866	6.442	-27.025	-8.557	1.00	63.94	N
ATOM	1477	CA	SER	A	866	6.744	-25.637	-8.839	1.00	61.06	C
ATOM	1478	C	SER	A	866	6.030	-24.646	-7.929	1.00	59.17	C
ATOM	1479	O	SER	A	866	6.735	-23.771	-7.443	1.00	58.24	O
ATOM	1480	CB	SER	A	866	6.496	-25.465	-10.338	1.00	58.29	C
ATOM	1481	OG	SER	A	866	5.098	-25.671	-10.413	1.00	56.88	O
ATOM	1482	N	SER	A	867	4.756	-24.695	-7.655	1.00	57.42	N
ATOM	1483	CA	SER	A	867	4.027	-23.973	-6.663	1.00	56.08	C
ATOM	1484	C	SER	A	867	4.622	-24.050	-5.253	1.00	56.19	C
ATOM	1485	O	SER	A	867	4.886	-23.066	-4.535	1.00	57.44	O
ATOM	1486	CB	SER	A	867	2.606	-24.544	-6.576	1.00	55.54	C
ATOM	1487	OG	SER	A	867	1.601	-23.753	-7.180	1.00	55.69	O
ATOM	1488	N	GLN	A	868	4.932	-25.254	-4.775	1.00	53.04	N
ATOM	1489	CA	GLN	A	868	5.169	-25.426	-3.345	1.00	50.22	C
ATOM	1490	C	GLN	A	868	6.537	-24.791	-3.098	1.00	45.43	C
ATOM	1491	O	GLN	A	868	6.820	-24.208	-2.064	1.00	42.26	O
ATOM	1492	CB	GLN	A	868	4.939	-26.881	-2.967	1.00	53.14	C
ATOM	1493	CG	GLN	A	868	3.569	-27.507	-2.880	1.00	56.67	C
ATOM	1494	CD	GLN	A	868	3.277	-28.988	-2.957	1.00	59.47	C
ATOM	1495	OE1	GLN	A	868	3.459	-29.857	-2.052	1.00	61.09	O
ATOM	1496	NE2	GLN	A	868	2.745	-29.482	-4.085	1.00	58.57	N
ATOM	1497	N	ARG	A	869	7.399	-24.844	-4.098	1.00	39.95	N
ATOM	1498	CA	ARG	A	869	8.751	-24.389	-4.243	1.00	33.44	C
ATOM	1499	C	ARG	A	869	8.789	-22.875	-4.150	1.00	33.09	C
ATOM	1500	O	ARG	A	869	9.556	-22.418	-3.364	1.00	31.40	O
ATOM	1501	CB	ARG	A	869	9.321	-24.744	-5.614	1.00	25.35	C
ATOM	1502	CG	ARG	A	869	10.768	-24.915	-5.902	1.00	19.22	C
ATOM	1503	CD	ARG	A	869	11.753	-25.374	-4.838	1.00	13.37	C
ATOM	1504	NE	ARG	A	869	13.131	-25.065	-5.049	1.00	7.23	N
ATOM	1505	CZ	ARG	A	869	14.271	-25.386	-4.547	1.00	10.82	C
ATOM	1506	NH1	ARG	A	869	14.575	-26.236	-3.530	1.00	9.93	N
ATOM	1507	NH2	ARG	A	869	15.455	-24.880	-5.019	1.00	13.47	N
ATOM	1508	N	PHE	A	870	7.952	-22.245	-4.950	1.00	34.01	N
ATOM	1509	CA	PHE	A	870	7.650	-20.858	-4.892	1.00	35.86	C
ATOM	1510	C	PHE	A	870	7.256	-20.486	-3.456	1.00	40.16	C
ATOM	1511	O	PHE	A	870	7.818	-19.621	-2.796	1.00	40.44	O
ATOM	1512	CB	PHE	A	870	6.574	-20.418	-5.833	1.00	29.79	C
ATOM	1513	CG	PHE	A	870	6.345	-18.903	-5.906	1.00	27.56	C
ATOM	1514	CD1	PHE	A	870	7.104	-18.105	-6.749	1.00	23.45	C
ATOM	1515	CD2	PHE	A	870	5.348	-18.307	-5.148	1.00	25.73	C
ATOM	1516	CE1	PHE	A	870	6.893	-16.786	-6.813	1.00	23.43	C
ATOM	1517	CE2	PHE	A	870	5.128	-16.972	-5.229	1.00	25.96	C
ATOM	1518	CZ	PHE	A	870	5.921	-16.177	-6.045	1.00	25.00	C
ATOM	1519	N	TYR	A	871	6.299	-21.181	-2.893	1.00	45.62	N
ATOM	1520	CA	TYR	A	871	5.827	-20.968	-1.548	1.00	48.82	C
ATOM	1521	C	TYR	A	871	7.069	-20.963	-0.664	1.00	47.49	C
ATOM	1522	O	TYR	A	871	7.166	-20.059	0.150	1.00	46.54	O
ATOM	1523	CB	TYR	A	871	4.872	-22.093	-1.119	1.00	51.16	C
ATOM	1524	CG	TYR	A	871	4.526	-21.924	0.342	1.00	54.43	C
ATOM	1525	CD1	TYR	A	871	5.402	-22.524	1.255	1.00	55.72	CD2 C
ATOM	1526	CD2	TYR	A	871	3.451	-21.189	0.800	1.00	54.29	CD1 C
ATOM	1527	CE1	TYR	A	871	5.175	-22.394	2.605	1.00	57.51	CE2 C
ATOM	1528	CE2	TYR	A	871	3.240	-21.079	2.154	1.00	56.19	CE1 C
ATOM	1529	CZ	TYR	A	871	4.091	-21.656	3.070	1.00	57.76	C
ATOM	1530	OH	TYR	A	871	3.968	-21.600	4.464	1.00	58.46	O
ATOM	1531	N	GLN	A	872	7.880	-21.967	-0.807	1.00	46.06	N
ATOM	1532	CA	GLN	A	872	9.050	-22.227	-0.018	1.00	45.90	C
ATOM	1533	C	GLN	A	872	10.214	-21.273	-0.150	1.00	43.41	C
ATOM	1534	O	GLN	A	872	10.937	-20.992	0.781	1.00	43.52	O
ATOM	1535	CB	GLN	A	872	9.613	-23.543	-0.604	1.00	48.52	C
ATOM	1536	CG	GLN	A	872	8.806	-24.765	-0.225	1.00	51.25	C
ATOM	1537	CD	GLN	A	872	9.640	-26.015	-0.283	1.00	52.73	C

FIG. 7 CONT'D

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ATOM   1538  OE1 GLN A 872       9.933 -26.513  -1.393  1.00 53.86           O
ATOM   1539  NE2 GLN A 872       9.918 -26.370   0.974  1.00 53.69           N
ATOM   1540  N   LEU A 873      10.452 -20.862  -1.385  1.00 39.03           N
ATOM   1541  CA  LEU A 873      11.441 -19.842  -1.654  1.00 32.93           C
ATOM   1542  C   LEU A 873      10.967 -18.458  -1.242  1.00 35.35           C
ATOM   1543  O   LEU A 873      11.841 -17.717  -0.759  1.00 37.08           O
ATOM   1544  CB  LEU A 873      11.996 -19.904  -3.048  1.00 20.49           C
ATOM   1545  CG  LEU A 873      12.795 -21.171  -3.332  1.00 14.67           C
ATOM   1546  CD1 LEU A 873      13.482 -21.079  -4.691  1.00  3.70           C
ATOM   1547  CD2 LEU A 873      13.884 -21.509  -2.340  1.00 10.81           C
ATOM   1548  N   THR A 874       9.674 -18.172  -1.280  1.00 36.48           N
ATOM   1549  CA  THR A 874       9.133 -16.984  -0.606  1.00 37.02           C
ATOM   1550  C   THR A 874       8.979 -17.082   0.898  1.00 38.39           C
ATOM   1551  O   THR A 874       9.614 -16.191   1.499  1.00 39.53           O
ATOM   1552  CB  THR A 874       7.876 -16.462  -1.285  1.00 34.81           C
ATOM   1553  OG1 THR A 874       6.747 -17.345  -1.291  1.00 34.06           O
ATOM   1554  CG2 THR A 874       8.254 -16.159  -2.729  1.00 35.07           C
ATOM   1555  N   LYS A 875       8.405 -17.979   1.667  1.00 38.00           N
ATOM   1556  CA  LYS A 875       8.628 -18.043   3.102  1.00 38.82           C
ATOM   1557  C   LYS A 875      10.084 -17.841   3.508  1.00 37.54           C
ATOM   1558  O   LYS A 875      10.396 -17.256   4.544  1.00 36.71           O
ATOM   1559  CB  LYS A 875       8.209 -19.362   3.690  1.00 38.28           C
ATOM   1560  CG  LYS A 875       7.481 -19.545   4.983  1.00 38.75           C
ATOM   1561  CD  LYS A 875       6.439 -18.461   5.195  1.00 40.72           C
ATOM   1562  CE  LYS A 875       5.715 -18.603   6.532  1.00 41.02           C
ATOM   1563  NZ  LYS A 875       4.847 -17.394   6.820  1.00 41.32           N
ATOM   1564  N   LEU A 876      11.075 -18.299   2.783  1.00 35.77           N
ATOM   1565  CA  LEU A 876      12.478 -18.265   3.180  1.00 35.39           C
ATOM   1566  C   LEU A 876      12.865 -16.793   3.259  1.00 37.16           C
ATOM   1567  O   LEU A 876      13.650 -16.389   4.099  1.00 39.31           O
ATOM   1568  CB  LEU A 876      13.428 -18.905   2.185  1.00 29.75           C
ATOM   1569  CG  LEU A 876      14.858 -19.242   2.484  1.00 26.77           C
ATOM   1570  CD1 LEU A 876      15.519 -19.960   1.268  1.00 27.43           C
ATOM   1571  CD2 LEU A 876      15.791 -18.174   2.889  1.00 22.70           C
ATOM   1572  N   LEU A 877      12.422 -16.040   2.261  1.00 35.97           N
ATOM   1573  CA  LEU A 877      12.638 -14.617   2.316  1.00 34.49           C
ATOM   1574  C   LEU A 877      11.842 -13.939   3.410  1.00 34.55           C
ATOM   1575  O   LEU A 877      12.371 -13.062   4.049  1.00 34.73           O
ATOM   1576  CB  LEU A 877      12.158 -14.117   0.967  1.00 30.93           C
ATOM   1577  CG  LEU A 877      13.137 -14.183  -0.175  1.00 27.55           C
ATOM   1578  CD1 LEU A 877      12.305 -13.328  -1.121  1.00 29.91           C
ATOM   1579  CD2 LEU A 877      14.499 -13.578  -0.027  1.00 27.14           C
ATOM   1580  N   ASP A 878      10.579 -14.256   3.591  1.00 35.63           N
ATOM   1581  CA  ASP A 878       9.653 -13.696   4.541  1.00 36.21           C
ATOM   1582  C   ASP A 878      10.266 -13.871   5.942  1.00 37.33           C
ATOM   1583  O   ASP A 878      10.129 -13.042   6.835  1.00 36.34           O
ATOM   1584  CB  ASP A 878       8.254 -14.213   4.555  1.00 34.71           C
ATOM   1585  CG  ASP A 878       6.974 -13.984   3.851  1.00 35.27           C
ATOM   1586  OD1 ASP A 878       6.675 -13.132   3.027  1.00 31.61           O
ATOM   1587  OD2 ASP A 878       5.935 -14.724   4.072  1.00 37.93           O
ATOM   1588  N   ASN A 879      10.929 -15.007   6.125  1.00 38.67           N
ATOM   1589  CA  ASN A 879      11.667 -15.353   7.296  1.00 39.18           C
ATOM   1590  C   ASN A 879      12.925 -14.588   7.634  1.00 41.48           C
ATOM   1591  O   ASN A 879      13.253 -14.603   8.812  1.00 44.06           O
ATOM   1592  CB  ASN A 879      12.167 -16.814   7.116  1.00 33.55           C
ATOM   1593  CG  ASN A 879      11.093 -17.722   7.652  1.00 27.79           C
ATOM   1594  OD1 ASN A 879      10.136 -17.133   8.106  1.00 22.37           O
ATOM   1595  ND2 ASN A 879      11.455 -18.980   7.497  1.00 26.73           N
ATOM   1596  N   LEU A 880      13.705 -14.051   6.709  1.00 41.27           N
ATOM   1597  CA  LEU A 880      14.923 -13.360   7.079  1.00 40.26           C
ATOM   1598  C   LEU A 880      14.584 -11.969   7.583  1.00 40.54           C
ATOM   1599  O   LEU A 880      15.531 -11.410   8.085  1.00 40.48           O
ATOM   1600  CB  LEU A 880      16.061 -13.177   6.116  1.00 39.66           C
ATOM   1601  CG  LEU A 880      16.473 -14.186   5.054  1.00 39.47           C
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FIG. 7 CONT'D

ATOM	1602	CD1	LEU	A	880	17.127	-13.478	3.861	1.00	40.05	C
ATOM	1603	CD2	LEU	A	880	17.459	-15.206	5.530	1.00	35.80	C
ATOM	1604	N	HIS	A	881	13.415	-11.420	7.530	1.00	42.52	N
ATOM	1605	CA	HIS	A	881	13.143	-10.221	8.284	1.00	46.26	C
ATOM	1606	C	HIS	A	881	13.705	-10.389	9.709	1.00	46.68	C
ATOM	1607	O	HIS	A	881	14.737	-9.823	10.106	1.00	46.39	O
ATOM	1608	CB	HIS	A	881	11.672	-9.801	8.181	1.00	48.04	C
ATOM	1609	CG	HIS	A	881	11.242	-9.276	6.856	1.00	51.27	C
ATOM	1610	ND1	HIS	A	881	10.002	-9.537	6.304	1.00	53.31	N
ATOM	1611	CD2	HIS	A	881	11.876	-8.536	5.918	1.00	52.37	C
ATOM	1612	CE1	HIS	A	881	9.882	-8.972	5.106	1.00	53.29	C
ATOM	1613	NE2	HIS	A	881	11.019	-8.359	4.842	1.00	53.03	N
ATOM	1614	N	ASP	A	882	13.022	-11.214	10.494	1.00	45.15	N
ATOM	1615	CA	ASP	A	882	13.293	-11.430	11.858	1.00	41.67	C
ATOM	1616	C	ASP	A	882	14.733	-11.742	12.096	1.00	38.20	C
ATOM	1617	O	ASP	A	882	15.245	-11.020	12.947	1.00	37.54	O
ATOM	1618	CB	ASP	A	882	12.587	-12.571	12.521	1.00	44.81	C
ATOM	1619	CG	ASP	A	882	11.341	-11.937	13.131	1.00	47.74	C
ATOM	1620	OD1	ASP	A	882	11.071	-10.868	12.578	1.00	45.85	O
ATOM	1621	OD2	ASP	A	882	10.840	-12.586	14.074	1.00	51.36	O
ATOM	1622	N	LEU	A	883	15.267	-12.689	11.371	1.00	33.45	N
ATOM	1623	CA	LEU	A	883	16.739	-12.882	11.457	1.00	30.06	C
ATOM	1624	C	LEU	A	883	17.566	-11.613	11.281	1.00	30.51	C
ATOM	1625	O	LEU	A	883	18.363	-11.290	12.159	1.00	31.62	O
ATOM	1626	CB	LEU	A	883	17.092	-13.991	10.500	1.00	23.12	C
ATOM	1627	CG	LEU	A	883	18.452	-14.653	10.430	1.00	19.32	C
ATOM	1628	CD1	LEU	A	883	18.393	-15.625	9.243	1.00	16.29	C
ATOM	1629	CD2	LEU	A	883	19.591	-13.658	10.239	1.00	16.61	C
ATOM	1630	N	VAL	A	884	17.423	-10.799	10.244	1.00	27.74	N
ATOM	1631	CA	VAL	A	884	17.920	-9.474	10.073	1.00	24.98	C
ATOM	1632	C	VAL	A	884	17.713	-8.521	11.250	1.00	24.82	C
ATOM	1633	O	VAL	A	884	18.602	-7.705	11.585	1.00	21.40	O
ATOM	1634	CB	VAL	A	884	17.436	-8.868	8.724	1.00	21.33	C
ATOM	1635	CG1	VAL	A	884	17.547	-7.339	8.655	1.00	17.84	C
ATOM	1636	CG2	VAL	A	884	18.389	-9.417	7.666	1.00	17.62	C
ATOM	1637	N	LYS	A	885	16.561	-8.554	11.927	1.00	23.69	N
ATOM	1638	CA	LYS	A	885	16.327	-7.570	12.987	1.00	23.16	C
ATOM	1639	C	LYS	A	885	17.199	-7.821	14.219	1.00	25.36	C
ATOM	1640	O	LYS	A	885	17.369	-7.039	15.114	1.00	25.04	O
ATOM	1641	CB	LYS	A	885	14.832	-7.511	13.288	1.00	17.69	C
ATOM	1642	CG	LYS	A	885	14.644	-6.952	14.681	1.00	16.12	C
ATOM	1643	CD	LYS	A	885	13.260	-6.942	15.167	1.00	16.34	C
ATOM	1644	CE	LYS	A	885	12.733	-5.547	15.538	1.00	16.64	C
ATOM	1645	NZ	LYS	A	885	11.437	-5.963	16.147	1.00	18.52	N
ATOM	1646	N	GLN	A	886	17.745	-9.010	14.348	1.00	27.66	N
ATOM	1647	CA	GLN	A	886	18.819	-9.388	15.175	1.00	29.52	C
ATOM	1648	C	GLN	A	886	20.190	-8.959	14.715	1.00	29.00	C
ATOM	1649	O	GLN	A	886	20.922	-8.404	15.553	1.00	30.15	O
ATOM	1650	CB	GLN	A	886	18.753	-10.904	15.393	1.00	30.29	C
ATOM	1651	CG	GLN	A	886	17.607	-11.351	16.283	1.00	29.73	C
ATOM	1652	CD	GLN	A	886	17.492	-12.809	15.972	1.00	33.11	C
ATOM	1653	OE1	GLN	A	886	18.457	-13.318	15.386	1.00	34.55	O
ATOM	1654	NE2	GLN	A	886	16.389	-13.447	16.344	1.00	35.15	N
ATOM	1655	N	LEU	A	887	20.589	-9.152	13.452	1.00	25.62	N
ATOM	1656	CA	LEU	A	887	21.852	-8.496	13.079	1.00	20.99	C
ATOM	1657	C	LEU	A	887	21.711	-7.047	13.524	1.00	20.49	C
ATOM	1658	O	LEU	A	887	22.622	-6.375	13.935	1.00	19.71	O
ATOM	1659	CB	LEU	A	887	22.177	-8.710	11.606	1.00	13.43	C
ATOM	1660	CG	LEU	A	887	22.158	-10.075	10.981	1.00	11.63	C
ATOM	1661	CD1	LEU	A	887	22.825	-10.489	9.673	1.00	8.22	C
ATOM	1662	CD2	LEU	A	887	22.729	-11.040	12.033	1.00	15.72	C
ATOM	1663	N	HIS	A	888	20.600	-6.369	13.279	1.00	19.79	N
ATOM	1664	CA	HIS	A	888	20.375	-4.939	13.171	1.00	18.36	C
ATOM	1665	C	HIS	A	888	20.647	-4.226	14.502	1.00	16.84	C

FIG. 7 CONT'D

ATOM	1666	O	HIS	A	888	21.381	-3.288	14.792	1.00	5.76	O
ATOM	1667	CB	HIS	A	888	18.964	-4.727	12.581	1.00	16.36	C
ATOM	1668	CG	HIS	A	888	18.765	-4.466	11.104	1.00	13.31	C
ATOM	1669	ND1	HIS	A	888	17.520	-4.633	10.339	1.00	10.67	N
ATOM	1670	CD2	HIS	A	888	19.762	-4.015	10.278	1.00	6.29	C
ATOM	1671	CE1	HIS	A	888	17.816	-4.303	9.119	1.00	7.44	C
ATOM	1672	NE2	HIS	A	888	19.128	-3.961	9.041	1.00	2.62	N
ATOM	1673	N	LEU	A	889	19.958	-4.759	15.510	1.00	18.47	N
ATOM	1674	CA	LEU	A	889	20.055	-4.513	16.929	1.00	19.13	C
ATOM	1675	C	LEU	A	889	21.396	-4.813	17.564	1.00	17.06	C
ATOM	1676	O	LEU	A	889	21.859	-3.884	18.283	1.00	16.78	O
ATOM	1677	CB	LEU	A	889	18.913	-5.149	17.688	1.00	18.40	C
ATOM	1678	CG	LEU	A	889	19.224	-5.062	19.198	1.00	21.45	C
ATOM	1679	CD1	LEU	A	889	19.309	-3.626	19.664	1.00	16.66	C
ATOM	1680	CD2	LEU	A	889	18.202	-6.043	19.824	1.00	22.03	C
ATOM	1681	N	TYR	A	890	22.023	-5.862	17.152	1.00	15.56	N
ATOM	1682	CA	TYR	A	890	23.437	-6.139	17.374	1.00	15.96	C
ATOM	1683	C	TYR	A	890	24.415	-5.113	16.793	1.00	16.33	C
ATOM	1684	O	TYR	A	890	25.471	-4.858	17.406	1.00	14.00	O
ATOM	1685	CB	TYR	A	890	23.826	-7.562	16.881	1.00	15.77	C
ATOM	1686	CG	TYR	A	890	25.245	-7.979	17.097	1.00	17.22	C
ATOM	1687	CD1	TYR	A	890	26.316	-7.692	16.282	1.00	14.60	C
ATOM	1688	CD2	TYR	A	890	25.493	-8.738	18.274	1.00	19.91	C
ATOM	1689	CE1	TYR	A	890	27.594	-8.057	16.583	1.00	16.54	C
ATOM	1690	CE2	TYR	A	890	26.766	-9.231	18.559	1.00	17.70	C
ATOM	1691	CZ	TYR	A	890	27.793	-8.855	17.733	1.00	18.76	C
ATOM	1692	OH	TYR	A	890	29.042	-9.309	18.033	1.00	18.92	O
ATOM	1693	N	CYS	A	891	24.127	-4.570	15.581	1.00	16.81	N
ATOM	1694	CA	CYS	A	891	25.036	-3.728	14.834	1.00	16.15	C
ATOM	1695	C	CYS	A	891	24.857	-2.289	15.396	1.00	17.16	C
ATOM	1696	O	CYS	A	891	25.831	-1.517	15.535	1.00	13.72	O
ATOM	1697	CB	CYS	A	891	24.933	-3.898	13.291	1.00	14.24	C
ATOM	1698	SG	CYS	A	891	25.867	-2.681	12.211	1.00	5.57	S
ATOM	1699	N	LEU	A	892	23.598	-2.012	15.802	1.00	15.79	N
ATOM	1700	CA	LEU	A	892	23.518	-0.685	16.435	1.00	19.87	C
ATOM	1701	C	LEU	A	892	24.201	-0.577	17.820	1.00	20.73	C
ATOM	1702	O	LEU	A	892	24.921	0.365	18.125	1.00	16.27	O
ATOM	1703	CB	LEU	A	892	22.084	-0.149	16.289	1.00	17.85	C
ATOM	1704	CG	LEU	A	892	22.016	1.317	16.821	1.00	19.82	C
ATOM	1705	CD1	LEU	A	892	22.648	2.461	16.013	1.00	17.22	C
ATOM	1706	CD2	LEU	A	892	20.563	1.591	17.163	1.00	19.67	C
ATOM	1707	N	ASN	A	893	24.000	-1.586	18.691	1.00	20.06	N
ATOM	1708	CA	ASN	A	893	24.632	-1.571	19.992	1.00	20.07	C
ATOM	1709	C	ASN	A	893	26.121	-1.795	19.824	1.00	20.53	C
ATOM	1710	O	ASN	A	893	26.764	-1.211	20.663	1.00	20.20	O
ATOM	1711	CB	ASN	A	893	24.193	-2.665	20.957	1.00	17.51	C
ATOM	1712	CG	ASN	A	893	22.724	-2.654	21.361	1.00	14.61	C
ATOM	1713	OD1	ASN	A	893	22.054	-1.618	21.442	1.00	14.24	O
ATOM	1714	ND2	ASN	A	893	22.287	-3.873	21.597	1.00	7.39	N
ATOM	1715	N	THR	A	894	26.704	-2.539	18.902	1.00	19.64	N
ATOM	1716	CA	THR	A	894	28.168	-2.378	18.772	1.00	17.66	C
ATOM	1717	C	THR	A	894	28.573	-1.025	18.229	1.00	20.84	C
ATOM	1718	O	THR	A	894	29.719	-0.651	18.332	1.00	18.92	O
ATOM	1719	CB	THR	A	894	28.763	-3.394	17.814	1.00	12.65	C
ATOM	1720	OG1	THR	A	894	28.318	-4.660	18.126	1.00	9.56	O
ATOM	1721	CG2	THR	A	894	30.250	-3.434	17.693	1.00	9.83	C
ATOM	1722	N	PHE	A	895	27.665	-0.401	17.442	1.00	25.02	N
ATOM	1723	CA	PHE	A	895	27.869	0.952	16.938	1.00	25.64	C
ATOM	1724	C	PHE	A	895	28.120	1.943	18.075	1.00	24.42	C
ATOM	1725	O	PHE	A	895	29.259	2.162	18.373	1.00	21.66	O
ATOM	1726	CB	PHE	A	895	26.703	1.514	16.100	1.00	22.07	C
ATOM	1727	CG	PHE	A	895	27.166	2.723	15.354	1.00	16.70	C
ATOM	1728	CD1	PHE	A	895	28.426	2.835	14.871	1.00	17.66	C
ATOM	1729	CD2	PHE	A	895	26.299	3.727	15.137	1.00	17.61	C

FIG. 7 CONT'D

ATOM	1730	CE1	PHE	A	895	28.858	3.933	14.181	1.00	19.61	C
ATOM	1731	CE2	PHE	A	895	26.720	4.869	14.479	1.00	18.61	C
ATOM	1732	CZ	PHE	A	895	28.004	5.007	13.991	1.00	18.04	C
ATOM	1733	N	ILE	A	896	27.051	2.395	18.654	1.00	25.58	N
ATOM	1734	CA	ILE	A	896	26.964	3.028	19.915	1.00	27.82	C
ATOM	1735	C	ILE	A	896	28.023	2.639	20.914	1.00	29.47	C
ATOM	1736	O	ILE	A	896	28.637	3.606	21.366	1.00	26.02	O
ATOM	1737	CB	ILE	A	896	25.528	2.860	20.444	1.00	26.96	C
ATOM	1738	CG1	ILE	A	896	24.611	3.566	19.446	1.00	26.08	C
ATOM	1739	CG2	ILE	A	896	25.300	3.475	21.810	1.00	28.88	C
ATOM	1740	CD1	ILE	A	896	23.192	3.158	19.693	1.00	26.13	C
ATOM	1741	N	GLN	A	897	28.357	1.427	21.347	1.00	31.97	N
ATOM	1742	CA	GLN	A	897	29.505	1.148	22.214	1.00	33.91	C
ATOM	1743	C	GLN	A	897	30.857	0.924	21.576	1.00	34.80	C
ATOM	1744	O	GLN	A	897	31.750	0.304	22.140	1.00	34.42	O
ATOM	1745	CB	GLN	A	897	29.125	-0.030	23.137	1.00	32.68	C
ATOM	1746	CG	GLN	A	897	27.667	-0.045	23.479	1.00	33.94	C
ATOM	1747	CD	GLN	A	897	26.690	-1.188	23.606	1.00	35.82	C
ATOM	1748	OE1	GLN	A	897	25.489	-0.954	23.197	1.00	37.08	O
ATOM	1749	NE2	GLN	A	897	26.942	-2.410	24.091	1.00	33.32	N
ATOM	1750	N	SER	A	898	31.163	1.487	20.416	1.00	35.40	N
ATOM	1751	CA	SER	A	898	32.306	1.129	19.575	1.00	34.27	C
ATOM	1752	C	SER	A	898	33.621	1.444	20.274	1.00	33.79	C
ATOM	1753	O	SER	A	898	34.651	0.854	20.004	1.00	34.20	O
ATOM	1754	CB	SER	A	898	32.263	1.727	18.146	1.00	31.15	C
ATOM	1755	OG	SER	A	898	33.135	2.792	17.777	1.00	25.99	O
ATOM	1756	N	ARG	A	899	33.694	2.427	21.112	1.00	36.10	N
ATOM	1757	CA	ARG	A	899	34.880	3.063	21.611	1.00	40.55	C
ATOM	1758	C	ARG	A	899	35.302	2.387	22.899	1.00	41.58	C
ATOM	1759	O	ARG	A	899	36.448	2.315	23.315	1.00	40.05	O
ATOM	1760	CB	ARG	A	899	34.610	4.504	22.045	1.00	43.30	C
ATOM	1761	CG	ARG	A	899	34.555	5.293	20.720	1.00	48.60	C
ATOM	1762	CD	ARG	A	899	35.919	5.125	20.014	1.00	50.16	C
ATOM	1763	NE	ARG	A	899	36.634	6.323	20.159	1.00	53.41	N
ATOM	1764	CZ	ARG	A	899	36.867	7.480	19.590	1.00	54.64	C
ATOM	1765	NH1	ARG	A	899	36.429	7.838	18.397	1.00	52.95	N
ATOM	1766	NH2	ARG	A	899	37.618	8.112	20.532	1.00	55.40	N
ATOM	1767	N	ALA	A	900	34.181	1.975	23.506	1.00	41.09	N
ATOM	1768	CA	ALA	A	900	34.280	1.012	24.594	1.00	40.63	C
ATOM	1769	C	ALA	A	900	34.949	-0.214	23.995	1.00	40.93	C
ATOM	1770	O	ALA	A	900	36.104	-0.513	24.210	1.00	41.65	O
ATOM	1771	CB	ALA	A	900	32.870	0.667	25.010	1.00	38.87	C
ATOM	1772	N	LEU	A	901	34.183	-0.744	23.046	1.00	39.67	N
ATOM	1773	CA	LEU	A	901	34.424	-1.942	22.307	1.00	35.57	C
ATOM	1774	C	LEU	A	901	35.693	-1.991	21.554	1.00	36.49	C
ATOM	1775	O	LEU	A	901	36.076	-3.136	21.292	1.00	38.81	O
ATOM	1776	CB	LEU	A	901	33.196	-2.198	21.381	1.00	29.43	C
ATOM	1777	CG	LEU	A	901	32.045	-2.570	22.328	1.00	26.15	C
ATOM	1778	CD1	LEU	A	901	30.663	-2.752	21.858	1.00	20.50	C
ATOM	1779	CD2	LEU	A	901	32.486	-3.810	23.145	1.00	25.71	C
ATOM	1780	N	SER	A	902	36.314	-0.904	21.173	1.00	36.40	N
ATOM	1781	CA	SER	A	902	37.503	-0.944	20.363	1.00	36.06	C
ATOM	1782	C	SER	A	902	37.262	-1.344	18.920	1.00	36.65	C
ATOM	1783	O	SER	A	902	38.161	-1.882	18.264	1.00	35.82	O
ATOM	1784	CB	SER	A	902	38.408	-2.005	20.995	1.00	30.77	C
ATOM	1785	OG	SER	A	902	39.468	-1.370	21.588	1.00	29.24	O
ATOM	1786	N	VAL	A	903	36.042	-1.237	18.444	1.00	36.56	N
ATOM	1787	CA	VAL	A	903	35.671	-1.627	17.089	1.00	36.56	C
ATOM	1788	C	VAL	A	903	35.512	-0.393	16.187	1.00	34.08	C
ATOM	1789	O	VAL	A	903	34.626	0.425	16.359	1.00	31.56	O
ATOM	1790	CB	VAL	A	903	34.302	-2.317	17.225	1.00	36.94	C
ATOM	1791	CG1	VAL	A	903	33.769	-2.627	15.836	1.00	38.13	C
ATOM	1792	CG2	VAL	A	903	34.451	-3.479	18.179	1.00	35.50	C
ATOM	1793	N	GLU	A	904	36.395	-0.250	15.258	1.00	29.98	N

FIG. 7 CONT'D

ATOM	1794	CA	GLU	A	904	36.224	0.586	14.108	1.00	31.30	C
ATOM	1795	C	GLU	A	904	35.155	0.179	13.074	1.00	28.97	C
ATOM	1796	O	GLU	A	904	35.214	-0.888	12.425	1.00	25.33	O
ATOM	1797	CB	GLU	A	904	37.686	0.582	13.756	1.00	28.65	C
ATOM	1798	CG	GLU	A	904	37.903	0.396	12.265	1.00	34.63	C
ATOM	1799	CD	GLU	A	904	38.516	1.709	11.850	1.00	39.48	C
ATOM	1800	OE1	GLU	A	904	39.310	2.054	12.796	1.00	42.78	O
ATOM	1801	OE2	GLU	A	904	38.001	2.134	10.787	1.00	38.73	O
ATOM	1802	N	PHE	A	905	34.094	1.047	12.981	1.00	24.49	N
ATOM	1803	CA	PHE	A	905	33.305	1.131	11.740	1.00	20.66	C
ATOM	1804	C	PHE	A	905	33.851	2.103	10.746	1.00	20.03	C
ATOM	1805	O	PHE	A	905	34.243	3.211	10.977	1.00	23.24	O
ATOM	1806	CB	PHE	A	905	31.849	1.427	12.043	1.00	12.08	C
ATOM	1807	CG	PHE	A	905	31.215	0.593	13.127	1.00	8.82	C
ATOM	1808	CD1	PHE	A	905	31.695	0.329	14.361	1.00	4.79	C
ATOM	1809	CD2	PHE	A	905	29.954	0.025	12.790	1.00	8.40	C
ATOM	1810	CE1	PHE	A	905	31.022	-0.587	15.157	1.00	2.02	C
ATOM	1811	CE2	PHE	A	905	29.290	-0.765	13.680	1.00	4.53	C
ATOM	1812	CZ	PHE	A	905	29.836	-1.116	14.922	1.00	5.24	C
ATOM	1813	N	PRO	A	906	34.066	1.821	9.492	1.00	20.31	N
ATOM	1814	CA	PRO	A	906	34.208	2.827	8.450	1.00	18.46	C
ATOM	1815	C	PRO	A	906	32.994	3.609	8.011	1.00	15.43	C
ATOM	1816	O	PRO	A	906	31.805	3.352	8.049	1.00	7.66	O
ATOM	1817	CB	PRO	A	906	34.923	2.087	7.366	1.00	16.88	C
ATOM	1818	CG	PRO	A	906	34.807	0.657	7.605	1.00	16.58	C
ATOM	1819	CD	PRO	A	906	34.066	0.440	8.904	1.00	18.64	C
ATOM	1820	N	GLU	A	907	33.416	4.733	7.445	1.00	17.27	N
ATOM	1821	CA	GLU	A	907	32.585	5.789	6.852	1.00	18.01	C
ATOM	1822	C	GLU	A	907	31.328	5.363	6.140	1.00	17.72	C
ATOM	1823	O	GLU	A	907	30.239	5.849	6.527	1.00	15.15	O
ATOM	1824	CB	GLU	A	907	33.508	6.637	5.993	1.00	13.55	C
ATOM	1825	CG	GLU	A	907	34.533	7.575	6.547	1.00	14.17	C
ATOM	1826	CD	GLU	A	907	34.048	8.321	7.793	1.00	12.46	C
ATOM	1827	OE1	GLU	A	907	32.901	8.799	7.879	1.00	14.83	O
ATOM	1828	OE2	GLU	A	907	34.630	8.531	8.804	1.00	8.29	O
ATOM	1829	N	MET	A	908	31.354	4.510	5.090	1.00	18.12	N
ATOM	1830	CA	MET	A	908	30.126	4.347	4.336	1.00	19.39	C
ATOM	1831	C	MET	A	908	29.056	3.704	5.141	1.00	21.26	C
ATOM	1832	O	MET	A	908	27.908	4.065	5.246	1.00	21.33	O
ATOM	1833	CB	MET	A	908	30.479	3.755	3.010	1.00	17.37	C
ATOM	1834	CG	MET	A	908	31.187	4.583	1.970	1.00	13.09	C
ATOM	1835	SD	MET	A	908	32.011	3.698	0.680	1.00	7.00	S
ATOM	1836	CE	MET	A	908	30.678	3.059	-0.256	1.00	12.32	C
ATOM	1837	N	MET	A	909	29.389	2.646	5.805	1.00	25.80	N
ATOM	1838	CA	MET	A	909	28.822	1.769	6.821	1.00	24.23	C
ATOM	1839	C	MET	A	909	28.278	2.521	8.003	1.00	22.03	C
ATOM	1840	O	MET	A	909	27.115	2.381	8.307	1.00	16.40	O
ATOM	1841	CB	MET	A	909	30.055	0.877	7.112	1.00	24.78	C
ATOM	1842	CG	MET	A	909	29.790	-0.597	7.111	1.00	27.30	C
ATOM	1843	SD	MET	A	909	29.881	-1.360	8.801	1.00	26.56	S
ATOM	1844	CE	MET	A	909	28.389	-2.341	8.595	1.00	24.79	C
ATOM	1845	N	SER	A	910	29.039	3.431	8.610	1.00	23.29	N
ATOM	1846	CA	SER	A	910	28.620	4.366	9.662	1.00	25.50	C
ATOM	1847	C	SER	A	910	27.386	5.240	9.374	1.00	26.34	C
ATOM	1848	O	SER	A	910	26.528	5.408	10.233	1.00	23.88	O
ATOM	1849	CB	SER	A	910	29.706	5.337	10.156	1.00	25.12	C
ATOM	1850	OG	SER	A	910	30.907	4.769	10.693	1.00	24.15	O
ATOM	1851	N	GLU	A	911	27.306	5.681	8.115	1.00	27.50	N
ATOM	1852	CA	GLU	A	911	26.323	6.604	7.579	1.00	27.09	C
ATOM	1853	C	GLU	A	911	25.030	5.880	7.372	1.00	24.23	C
ATOM	1854	O	GLU	A	911	24.171	6.346	8.078	1.00	18.58	O
ATOM	1855	CB	GLU	A	911	26.994	7.313	6.435	1.00	29.12	C
ATOM	1856	CG	GLU	A	911	26.432	8.369	5.579	1.00	33.01	C
ATOM	1857	CD	GLU	A	911	25.402	9.317	6.102	1.00	38.13	C

FIG. 7 CONT'D

ATOM	1858	OE1	GLU	A	911	25.405	9.848	7.228	1.00	38.93	O
ATOM	1859	OE2	GLU	A	911	24.372	9.688	5.453	1.00	42.57	O
ATOM	1860	N	VAL	A	912	25.051	4.756	6.636	1.00	23.34	N
ATOM	1861	CA	VAL	A	912	23.849	3.924	6.611	1.00	24.28	C
ATOM	1862	C	VAL	A	912	23.379	3.477	7.990	1.00	23.34	C
ATOM	1863	O	VAL	A	912	22.155	3.367	8.169	1.00	25.75	O
ATOM	1864	CB	VAL	A	912	23.744	2.827	5.551	1.00	22.68	C
ATOM	1865	CG1	VAL	A	912	23.783	3.462	4.162	1.00	26.21	C
ATOM	1866	CG2	VAL	A	912	24.840	1.816	5.277	1.00	22.42	C
ATOM	1867	N	ILE	A	913	24.176	3.191	8.950	1.00	20.79	N
ATOM	1868	CA	ILE	A	913	23.743	2.829	10.299	1.00	20.03	C
ATOM	1869	C	ILE	A	913	23.042	3.964	11.006	1.00	22.36	C
ATOM	1870	O	ILE	A	913	21.901	3.768	11.398	1.00	22.46	O
ATOM	1871	CB	ILE	A	913	24.932	2.228	11.122	1.00	14.83	C
ATOM	1872	CG1	ILE	A	913	25.490	0.938	10.520	1.00	12.36	C
ATOM	1873	CG2	ILE	A	913	24.711	1.968	12.589	1.00	2.02	C
ATOM	1874	CD1	ILE	A	913	26.984	0.850	10.842	1.00	16.15	C
ATOM	1875	N	ALA	A	914	23.680	5.089	11.260	1.00	25.32	N
ATOM	1876	CA	ALA	A	914	23.097	6.325	11.789	1.00	27.11	C
ATOM	1877	C	ALA	A	914	21.833	6.742	11.046	1.00	30.21	C
ATOM	1878	O	ALA	A	914	20.758	6.830	11.626	1.00	32.83	O
ATOM	1879	CB	ALA	A	914	24.112	7.461	11.703	1.00	21.54	C
ATOM	1880	N	ALA	A	915	21.915	6.906	9.723	1.00	30.85	N
ATOM	1881	CA	ALA	A	915	20.767	7.106	8.933	1.00	32.70	C
ATOM	1882	C	ALA	A	915	19.590	6.183	9.221	1.00	34.37	C
ATOM	1883	O	ALA	A	915	18.413	6.693	9.086	1.00	37.38	O
ATOM	1884	CB	ALA	A	915	21.216	6.949	7.473	1.00	34.98	C
ATOM	1885	N	GLN	A	916	19.706	4.839	9.289	1.00	32.65	N
ATOM	1886	CA	GLN	A	916	18.423	4.154	9.030	1.00	30.93	C
ATOM	1887	C	GLN	A	916	18.161	3.164	10.121	1.00	28.55	C
ATOM	1888	O	GLN	A	916	17.006	2.705	10.241	1.00	26.31	O
ATOM	1889	CB	GLN	A	916	18.366	3.777	7.565	1.00	31.46	C
ATOM	1890	CG	GLN	A	916	18.276	4.890	6.504	1.00	31.21	C
ATOM	1891	CD	GLN	A	916	16.939	5.562	6.444	1.00	31.77	C
ATOM	1892	OE1	GLN	A	916	16.134	5.412	7.375	1.00	32.55	O
ATOM	1893	NE2	GLN	A	916	16.578	6.255	5.367	1.00	31.42	N
ATOM	1894	N	LEU	A	917	19.168	2.951	11.002	1.00	24.99	N
ATOM	1895	CA	LEU	A	917	19.073	1.684	11.759	1.00	22.81	C
ATOM	1896	C	LEU	A	917	18.073	1.756	12.880	1.00	23.59	C
ATOM	1897	O	LEU	A	917	17.300	0.855	13.064	1.00	20.23	O
ATOM	1898	CB	LEU	A	917	20.415	1.192	12.208	1.00	18.96	C
ATOM	1899	CG	LEU	A	917	21.358	0.399	11.331	1.00	17.62	C
ATOM	1900	CD1	LEU	A	917	21.933	-0.799	12.082	1.00	14.54	C
ATOM	1901	CD2	LEU	A	917	20.707	-0.078	10.037	1.00	16.61	C
ATOM	1902	N	PRO	A	918	18.142	2.879	13.574	1.00	26.51	N
ATOM	1903	CA	PRO	A	918	17.193	3.228	14.618	1.00	29.42	C
ATOM	1904	C	PRO	A	918	15.751	3.234	14.222	1.00	33.31	C
ATOM	1905	O	PRO	A	918	14.973	2.433	14.722	1.00	36.26	O
ATOM	1906	CB	PRO	A	918	17.729	4.575	15.109	1.00	29.25	C
ATOM	1907	CG	PRO	A	918	19.168	4.659	14.726	1.00	26.78	C
ATOM	1908	CD	PRO	A	918	19.253	3.900	13.451	1.00	25.40	C
ATOM	1909	N	LYS	A	919	15.261	4.096	13.359	1.00	36.45	N
ATOM	1910	CA	LYS	A	919	14.099	3.977	12.478	1.00	36.49	C
ATOM	1911	C	LYS	A	919	13.701	2.582	11.971	1.00	33.16	C
ATOM	1912	O	LYS	A	919	12.592	2.077	12.230	1.00	32.62	O
ATOM	1913	CB	LYS	A	919	14.378	4.834	11.225	1.00	37.66	C
ATOM	1914	CG	LYS	A	919	13.313	4.770	10.175	1.00	40.37	C
ATOM	1915	CD	LYS	A	919	11.987	5.410	10.497	1.00	40.96	C
ATOM	1916	CE	LYS	A	919	11.840	6.825	9.948	1.00	40.67	C
ATOM	1917	NZ	LYS	A	919	10.584	7.272	10.619	1.00	39.50	N
ATOM	1918	N	ILE	A	920	14.626	1.902	11.287	1.00	27.98	N
ATOM	1919	CA	ILE	A	920	14.359	0.488	11.012	1.00	24.15	C
ATOM	1920	C	ILE	A	920	14.035	-0.263	12.272	1.00	22.06	C
ATOM	1921	O	ILE	A	920	12.984	-0.796	12.429	1.00	14.99	O

FIG. 7 CONT'D

ATOM	1922	CB	ILE	A	920	15.476	-0.173	10.207	1.00	21.22	C
ATOM	1923	CG1	ILE	A	920	15.502	0.380	8.777	1.00	16.13	C
ATOM	1924	CG2	ILE	A	920	15.366	-1.704	10.224	1.00	19.89	C
ATOM	1925	CD1	ILE	A	920	16.804	0.212	8.083	1.00	12.79	C
ATOM	1926	N	LEU	A	921	14.915	-0.209	13.243	1.00	26.75	N
ATOM	1927	CA	LEU	A	921	14.687	-0.974	14.485	1.00	32.12	C
ATOM	1928	C	LEU	A	921	13.470	-0.587	15.288	1.00	31.99	C
ATOM	1929	O	LEU	A	921	12.816	-1.473	15.843	1.00	32.66	O
ATOM	1930	CB	LEU	A	921	15.977	-1.006	15.305	1.00	31.35	C
ATOM	1931	CG	LEU	A	921	16.966	-2.034	14.722	1.00	33.33	C
ATOM	1932	CD1	LEU	A	921	18.293	-1.979	15.476	1.00	30.97	C
ATOM	1933	CD2	LEU	A	921	16.301	-3.433	14.591	1.00	29.77	C
ATOM	1934	N	ALA	A	922	13.058	0.647	15.306	1.00	30.08	N
ATOM	1935	CA	ALA	A	922	11.800	1.017	15.876	1.00	29.99	C
ATOM	1936	C	ALA	A	922	10.592	0.578	15.106	1.00	29.57	C
ATOM	1937	O	ALA	A	922	9.521	1.041	15.495	1.00	25.60	O
ATOM	1938	CB	ALA	A	922	11.764	2.554	16.051	1.00	31.57	C
ATOM	1939	N	GLY	A	923	10.723	-0.130	13.998	1.00	32.26	N
ATOM	1940	CA	GLY	A	923	9.701	-0.558	13.063	1.00	34.13	C
ATOM	1941	C	GLY	A	923	8.881	0.489	12.326	1.00	33.91	C
ATOM	1942	O	GLY	A	923	7.685	0.513	12.120	1.00	31.64	O
ATOM	1943	N	MET	A	924	9.593	1.554	12.016	1.00	34.89	N
ATOM	1944	CA	MET	A	924	9.010	2.671	11.259	1.00	36.87	C
ATOM	1945	C	MET	A	924	9.419	2.539	9.807	1.00	37.10	C
ATOM	1946	O	MET	A	924	10.035	3.358	9.196	1.00	36.68	O
ATOM	1947	CB	MET	A	924	9.355	3.914	12.073	1.00	36.10	C
ATOM	1948	CG	MET	A	924	9.171	3.776	13.582	1.00	35.63	C
ATOM	1949	SD	MET	A	924	7.844	4.584	14.470	1.00	34.34	S
ATOM	1950	CE	MET	A	924	6.391	4.284	13.524	1.00	33.30	C
ATOM	1951	N	VAL	A	925	9.234	1.423	9.142	1.00	37.57	N
ATOM	1952	CA	VAL	A	925	9.296	0.894	7.815	1.00	37.27	C
ATOM	1953	C	VAL	A	925	8.276	-0.232	7.541	1.00	37.22	C
ATOM	1954	O	VAL	A	925	7.751	-0.879	8.406	1.00	36.85	O
ATOM	1955	CB	VAL	A	925	10.598	0.264	7.268	1.00	36.56	C
ATOM	1956	CG1	VAL	A	925	11.742	1.268	7.309	1.00	37.65	C
ATOM	1957	CG2	VAL	A	925	11.029	-0.973	8.044	1.00	34.79	C
ATOM	1958	N	LYS	A	926	7.951	-0.408	6.282	1.00	38.06	N
ATOM	1959	CA	LYS	A	926	7.018	-1.371	5.733	1.00	38.97	C
ATOM	1960	C	LYS	A	926	7.818	-2.538	5.144	1.00	39.66	C
ATOM	1961	O	LYS	A	926	8.625	-2.528	4.216	1.00	38.47	O
ATOM	1962	CB	LYS	A	926	6.054	-0.778	4.720	1.00	37.21	C
ATOM	1963	CG	LYS	A	926	5.489	-1.622	3.609	1.00	35.09	C
ATOM	1964	CD	LYS	A	926	4.112	-1.106	3.192	1.00	35.78	C
ATOM	1965	CE	LYS	A	926	3.582	-1.599	1.857	1.00	35.42	C
ATOM	1966	NZ	LYS	A	926	2.443	-2.471	1.524	1.00	29.16	N
ATOM	1967	N	PRO	A	927	7.643	-3.658	5.833	1.00	39.28	N
ATOM	1968	CA	PRO	A	927	8.117	-4.936	5.316	1.00	40.90	C
ATOM	1969	C	PRO	A	927	7.130	-5.415	4.263	1.00	42.56	C
ATOM	1970	O	PRO	A	927	5.894	-5.369	4.460	1.00	43.54	O
ATOM	1971	CB	PRO	A	927	8.159	-5.804	6.541	1.00	38.81	C
ATOM	1972	CG	PRO	A	927	7.902	-4.906	7.697	1.00	36.83	C
ATOM	1973	CD	PRO	A	927	6.952	-3.879	7.126	1.00	37.73	C
ATOM	1974	N	LEU	A	928	7.671	-5.779	3.097	1.00	42.08	N
ATOM	1975	CA	LEU	A	928	6.789	-6.432	2.111	1.00	41.65	C
ATOM	1976	C	LEU	A	928	6.648	-7.902	2.479	1.00	42.29	C
ATOM	1977	O	LEU	A	928	7.622	-8.663	2.638	1.00	43.14	O
ATOM	1978	CB	LEU	A	928	7.268	-6.114	0.706	1.00	37.44	C
ATOM	1979	CG	LEU	A	928	7.317	-4.650	0.300	1.00	35.66	C
ATOM	1980	CD1	LEU	A	928	7.841	-4.537	-1.121	1.00	35.86	C
ATOM	1981	CD2	LEU	A	928	6.059	-3.819	0.458	1.00	32.47	C
ATOM	1982	N	LEU	A	929	5.424	-8.388	2.752	1.00	43.46	N
ATOM	1983	CA	LEU	A	929	5.382	-9.849	2.861	1.00	44.98	C
ATOM	1984	C	LEU	A	929	4.915	-10.564	1.618	1.00	45.47	C
ATOM	1985	O	LEU	A	929	3.859	-10.156	1.175	1.00	46.20	O

FIG. 7 CONT'D

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ATOM   1986  CB  LEU A 929       4.537 -10.270   4.052  1.00 44.54           C
ATOM   1987  CG  LEU A 929       5.074  -9.705   5.383  1.00 44.16           C
ATOM   1988  CD1 LEU A 929       4.020 -10.038   6.411  1.00 42.98           C
ATOM   1989  CD2 LEU A 929       6.492 -10.180   5.625  1.00 43.92           C
ATOM   1990  N   PHE A 930       5.574 -11.575   1.097  1.00 46.60           N
ATOM   1991  CA  PHE A 930       4.967 -12.698   0.375  1.00 48.74           C
ATOM   1992  C   PHE A 930       3.831 -13.476   1.066  1.00 53.82           C
ATOM   1993  O   PHE A 930       2.820 -13.692   0.370  1.00 52.34           O
ATOM   1994  CB  PHE A 930       6.002 -13.745  -0.132  1.00 39.00           C
ATOM   1995  CG  PHE A 930       6.856 -13.178  -1.209  1.00 33.12           C
ATOM   1996  CD1 PHE A 930       6.389 -12.853  -2.469  1.00 31.86           C
ATOM   1997  CD2 PHE A 930       8.179 -12.902  -1.007  1.00 31.21           C
ATOM   1998  CE1 PHE A 930       7.226 -12.263  -3.405  1.00 30.68           C
ATOM   1999  CE2 PHE A 930       9.002 -12.323  -1.953  1.00 28.86           C
ATOM   2000  CZ  PHE A 930       8.550 -11.980  -3.182  1.00 28.25           C
ATOM   2001  N   HIS A 931       3.888 -13.886   2.348  1.00 59.65           N
ATOM   2002  CA  HIS A 931       2.781 -14.578   2.983  1.00 65.43           C
ATOM   2003  C   HIS A 931       2.020 -13.952   4.132  1.00 67.22           C
ATOM   2004  O   HIS A 931       2.554 -13.045   4.767  1.00 69.36           O
ATOM   2005  CB  HIS A 931       3.295 -15.945   3.533  1.00 67.44           C
ATOM   2006  CG  HIS A 931       3.913 -16.719   2.399  1.00 69.16           C
ATOM   2007  ND1 HIS A 931       3.249 -16.876   1.188  1.00 69.39           N
ATOM   2008  CD2 HIS A 931       5.121 -17.305   2.269  1.00 69.70           C
ATOM   2009  CE1 HIS A 931       4.030 -17.532   0.366  1.00 69.72           C
ATOM   2010  NE2 HIS A 931       5.160 -17.824   0.989  1.00 70.09           N
ATOM   2011  N   LYS A 932       0.846 -14.480   4.543  1.00 66.01 >         N
ATOM   2012  CA  LYS A 932       0.010 -13.702   5.456  1.00 66.06 >         C
ATOM   2013  C   LYS A 932      -0.216 -14.347   6.814  1.00 65.79 >         C
ATOM   2014  O   LYS A 932      -1.294 -14.151   7.396  1.00 65.80 >         O
ATOM   2015  CB  LYS A 932      -1.310 -13.188   4.912  1.00 65.86 >         C
ATOM   2016  CG  LYS A 932      -2.152 -13.748   3.835  1.00 64.51 >         C
ATOM   2017  CD  LYS A 932      -2.956 -14.979   4.177  1.00 64.04 >         C
ATOM   2018  CE  LYS A 932      -2.289 -16.287   3.755  1.00 63.54 >         C
ATOM   2019  NZ  LYS A 932      -3.220 -17.242   3.092  1.00 62.38 >         N
TER    2020
ATOM   2021  N   LEU B 683      -8.296   9.571  54.281  1.00 60.73  <         N
ATOM   2022  CA  LEU B 683      -7.843  10.756  54.988  1.00 59.76  <         C
ATOM   2023  C   LEU B 683      -6.595  11.237  54.263  1.00 58.11  <         C
ATOM   2024  O   LEU B 683      -6.088  12.283  53.955  1.00 56.84  <         O
ATOM   2025  CB  LEU B 683      -7.488  10.378  56.418  1.00 61.68  <         C
ATOM   2026  CG  LEU B 683      -8.437  10.107  57.575  1.00 62.36  <         C
ATOM   2027  CD1 LEU B 683      -7.638   9.585  58.787  1.00 60.71  <         C
ATOM   2028  CD2 LEU B 683      -9.274  11.309  58.015  1.00 61.60  <         C
ATOM   2029  N   ILE B 684      -5.796  10.243  54.044  1.00 57.57           N
ATOM   2030  CA  ILE B 684      -4.775   9.988  53.099  1.00 54.74           C
ATOM   2031  C   ILE B 684      -4.169   8.700  53.702  1.00 51.51           C
ATOM   2032  O   ILE B 684      -3.675   8.691  54.797  1.00 51.24           O
ATOM   2033  CB  ILE B 684      -3.576  10.838  52.764  1.00 53.75           C
ATOM   2034  CG1 ILE B 684      -3.810  12.303  52.504  1.00 54.25           C
ATOM   2035  CG2 ILE B 684      -2.982  10.138  51.539  1.00 52.60           C
ATOM   2036  CD1 ILE B 684      -4.814  12.672  51.431  1.00 53.30           C
ATOM   2037  N   PRO B 685      -4.429   7.641  52.996  1.00 48.65           N
ATOM   2038  CA  PRO B 685      -3.673   6.435  53.077  1.00 47.42           C
ATOM   2039  C   PRO B 685      -2.197   6.695  53.294  1.00 46.85           C
ATOM   2040  O   PRO B 685      -1.533   7.412  52.560  1.00 46.88           O
ATOM   2041  CB  PRO B 685      -3.667   5.898  51.656  1.00 46.51           C
ATOM   2042  CG  PRO B 685      -4.746   6.651  50.993  1.00 46.71           C
ATOM   2043  CD  PRO B 685      -5.525   7.407  52.036  1.00 47.06           C
ATOM   2044  N   PRO B 686      -1.716   5.938  54.262  1.00 44.76           N
ATOM   2045  CA  PRO B 686      -0.359   6.063  54.741  1.00 41.82           C
ATOM   2046  C   PRO B 686       0.688   6.264  53.676  1.00 36.81           C
ATOM   2047  O   PRO B 686       1.494   7.202  53.708  1.00 35.66           O
ATOM   2048  CB  PRO B 686      -0.243   4.736  55.559  1.00 41.41           C
ATOM   2049  CG  PRO B 686      -1.587   4.620  56.216  1.00 40.30           C
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FIG. 7 CONT'D

ATOM	2050	CD	PRO	B	686	-2.490	4.912	55.044	1.00	43.14	C
ATOM	2051	N	LEU	B	687	0.767	5.394	52.711	1.00	32.10	N
ATOM	2052	CA	LEU	B	687	1.717	5.313	51.616	1.00	27.64	C
ATOM	2053	C	LEU	B	687	1.514	6.539	50.750	1.00	26.26	C
ATOM	2054	O	LEU	B	687	2.387	7.338	50.388	1.00	24.15	O
ATOM	2055	CB	LEU	B	687	1.422	4.016	50.952	1.00	20.64	C
ATOM	2056	CG	LEU	B	687	2.037	3.192	49.882	1.00	14.11	C
ATOM	2057	CD1	LEU	B	687	3.528	3.047	49.856	1.00	14.46	C
ATOM	2058	CD2	LEU	B	687	1.441	1.847	50.094	1.00	7.60	C
ATOM	2059	N	ILE	B	688	0.243	6.905	50.648	1.00	27.50	N
ATOM	2060	CA	ILE	B	688	0.015	8.187	49.941	1.00	27.62	C
ATOM	2061	C	ILE	B	688	0.725	9.280	50.695	1.00	28.13	C
ATOM	2062	O	ILE	B	688	1.473	9.983	50.006	1.00	28.59	O
ATOM	2063	CB	ILE	B	688	-1.395	8.408	49.415	1.00	25.00	C
ATOM	2064	CG1	ILE	B	688	-2.069	7.141	48.871	1.00	24.27	C
ATOM	2065	CG2	ILE	B	688	-1.332	9.235	48.149	1.00	23.02	C
ATOM	2066	CD1	ILE	B	688	-3.384	7.355	48.169	1.00	21.00	C
ATOM	2067	N	ASN	B	689	0.838	9.368	52.009	1.00	28.30	N
ATOM	2068	CA	ASN	B	689	1.644	10.457	52.563	1.00	30.00	C
ATOM	2069	C	ASN	B	689	3.128	10.317	52.365	1.00	31.11	C
ATOM	2070	O	ASN	B	689	3.789	11.342	52.253	1.00	27.30	O
ATOM	2071	CB	ASN	B	689	1.343	10.767	54.007	1.00	32.65	C
ATOM	2072	CG	ASN	B	689	-0.180	10.964	54.188	1.00	38.12	C
ATOM	2073	OD1	ASN	B	689	-0.964	11.781	53.515	1.00	36.44	O
ATOM	2074	ND2	ASN	B	689	-0.463	10.108	55.199	1.00	35.99	N
ATOM	2075	N	LEU	B	690	3.521	9.029	52.350	1.00	33.34	N
ATOM	2076	CA	LEU	B	690	4.912	8.654	52.201	1.00	31.60	C
ATOM	2077	C	LEU	B	690	5.286	8.962	50.759	1.00	30.60	C
ATOM	2078	O	LEU	B	690	6.312	9.626	50.592	1.00	32.27	O
ATOM	2079	CB	LEU	B	690	5.234	7.193	52.446	1.00	32.13	C
ATOM	2080	CG	LEU	B	690	6.737	6.871	52.518	1.00	32.78	C
ATOM	2081	CD1	LEU	B	690	7.265	7.159	53.951	1.00	34.77	C
ATOM	2082	CD2	LEU	B	690	7.028	5.444	52.187	1.00	29.32	C
ATOM	2083	N	LEU	B	691	4.360	8.674	49.816	1.00	26.45	* N
ATOM	2084	CA	LEU	B	691	4.822	9.119	48.491	1.00	24.45	* C
ATOM	2085	C	LEU	B	691	4.932	10.614	48.564	1.00	25.77	* C
ATOM	2086	O	LEU	B	691	6.042	11.030	48.282	1.00	23.93	* O
ATOM	2087	CB	LEU	B	691	4.211	8.439	47.292	1.00	20.00	* C
ATOM	2088	CG	LEU	B	691	4.354	6.906	47.307	1.00	14.87	* C
ATOM	2089	CD1	LEU	B	691	3.202	6.445	46.444	1.00	14.94	* C
ATOM	2090	CD2	LEU	B	691	5.702	6.418	46.906	1.00	10.37	* C
ATOM	2091	N	MET	B	692	3.975	11.371	49.096	1.00	30.53	N
ATOM	2092	CA	MET	B	692	4.213	12.819	49.147	1.00	34.53	C
ATOM	2093	C	MET	B	692	5.614	13.152	49.646	1.00	36.05	C
ATOM	2094	O	MET	B	692	6.451	13.526	48.836	1.00	38.02	O
ATOM	2095	CB	MET	B	692	3.161	13.750	49.763	1.00	33.29	C
ATOM	2096	CG	MET	B	692	3.381	15.169	49.216	1.00	35.54	C
ATOM	2097	SD	MET	B	692	3.038	15.555	47.446	1.00	37.10	S
ATOM	2098	CE	MET	B	692	4.651	15.916	46.719	1.00	35.00	C
ATOM	2099	N	SER	B	693	5.964	12.877	50.878	1.00	36.64	N
ATOM	2100	CA	SER	B	693	7.266	13.203	51.431	1.00	32.62	C
ATOM	2101	C	SER	B	693	8.519	12.747	50.741	1.00	29.65	C
ATOM	2102	O	SER	B	693	9.489	13.472	50.792	1.00	27.22	O
ATOM	2103	CB	SER	B	693	7.287	12.465	52.789	1.00	32.25	C
ATOM	2104	OG	SER	B	693	6.565	11.279	52.531	1.00	31.06	O
ATOM	2105	N	ILE	B	694	8.625	11.605	50.074	1.00	28.94	N
ATOM	2106	CA	ILE	B	694	9.866	11.221	49.437	1.00	26.20	C
ATOM	2107	C	ILE	B	694	10.062	11.914	48.129	1.00	29.35	C
ATOM	2108	O	ILE	B	694	11.144	11.823	47.605	1.00	30.95	O
ATOM	2109	CB	ILE	B	694	9.998	9.733	49.319	1.00	21.02	C
ATOM	2110	CG1	ILE	B	694	8.815	9.093	48.696	1.00	16.74	C
ATOM	2111	CG2	ILE	B	694	10.105	9.149	50.785	1.00	20.64	C
ATOM	2112	CD1	ILE	B	694	8.869	7.608	48.562	1.00	14.77	C
ATOM	2113	N	GLU	B	695	9.057	12.659	47.697	1.00	31.41	N

FIG. 7 CONT'D

ATOM	2114	CA	GLU	B	695	9.073	13.262	46.391	1.00	33.21	C
ATOM	2115	C	GLU	B	695	10.125	14.321	46.306	1.00	34.85	C
ATOM	2116	O	GLU	B	695	10.051	15.201	47.114	1.00	32.12	O
ATOM	2117	CB	GLU	B	695	7.656	13.780	46.240	1.00	31.35	C
ATOM	2118	CG	GLU	B	695	7.466	14.103	44.795	1.00	32.24	C
ATOM	2119	CD	GLU	B	695	7.510	12.932	43.855	1.00	29.22	C
ATOM	2120	OE1	GLU	B	695	6.974	11.876	44.088	1.00	27.97	O
ATOM	2121	OE2	GLU	B	695	8.110	13.087	42.809	1.00	31.34	O
ATOM	2122	N	PRO	B	696	11.059	14.227	45.392	1.00	37.47	N
ATOM	2123	CA	PRO	B	696	12.188	15.132	45.332	1.00	38.99	C
ATOM	2124	C	PRO	B	696	11.833	16.595	45.281	1.00	40.22	C
ATOM	2125	O	PRO	B	696	10.710	16.972	44.958	1.00	41.23	O
ATOM	2126	CB	PRO	B	696	12.940	14.741	44.058	1.00	39.14	C
ATOM	2127	CG	PRO	B	696	12.341	13.448	43.645	1.00	38.55	C
ATOM	2128	CD	PRO	B	696	10.895	13.489	44.092	1.00	37.48	C
ATOM	2129	N	ASP	B	697	12.811	17.444	45.493	1.00	42.13	N
ATOM	2130	CA	ASP	B	697	12.628	18.880	45.326	1.00	43.93	C
ATOM	2131	C	ASP	B	697	12.982	19.435	43.960	1.00	43.64	C
ATOM	2132	O	ASP	B	697	13.944	19.037	43.332	1.00	43.24	O
ATOM	2133	CB	ASP	B	697	13.630	19.605	46.245	1.00	44.28	C
ATOM	2134	CG	ASP	B	697	12.953	20.204	47.456	1.00	43.71	C
ATOM	2135	OD1	ASP	B	697	12.000	20.952	47.181	1.00	43.22	O
ATOM	2136	OD2	ASP	B	697	13.394	19.895	48.576	1.00	43.13	O
ATOM	2137	N	VAL	B	698	12.352	20.488	43.513	1.00	43.04	N
ATOM	2138	CA	VAL	B	698	12.305	20.988	42.145	1.00	42.14	C
ATOM	2139	C	VAL	B	698	13.723	21.145	41.649	1.00	38.95	C
ATOM	2140	O	VAL	B	698	14.664	21.376	42.389	1.00	40.22	O
ATOM	2141	CB	VAL	B	698	11.241	22.108	42.087	1.00	43.21	C
ATOM	2142	CG1	VAL	B	698	11.140	22.759	43.468	1.00	42.12	C
ATOM	2143	CG2	VAL	B	698	11.332	23.147	40.964	1.00	42.16	C
ATOM	2144	N	ILE	B	699	13.945	20.827	40.388	1.00	34.57	N
ATOM	2145	CA	ILE	B	699	15.228	20.642	39.759	1.00	29.06	C
ATOM	2146	C	ILE	B	699	15.368	21.761	38.730	1.00	29.62	C
ATOM	2147	O	ILE	B	699	14.615	21.680	37.760	1.00	28.70	O
ATOM	2148	CB	ILE	B	699	15.378	19.272	39.022	1.00	23.98	C
ATOM	2149	CG1	ILE	B	699	15.033	18.047	39.867	1.00	22.22	C
ATOM	2150	CG2	ILE	B	699	16.810	19.133	38.449	1.00	20.41	C
ATOM	2151	CD1	ILE	B	699	15.957	17.642	41.075	1.00	18.95	C
ATOM	2152	N	TYR	B	700	16.302	22.677	38.859	1.00	30.14	N
ATOM	2153	CA	TYR	B	700	16.698	23.541	37.792	1.00	33.03	C
ATOM	2154	C	TYR	B	700	17.424	22.915	36.631	1.00	33.84	C
ATOM	2155	O	TYR	B	700	18.127	21.920	36.804	1.00	35.81	O
ATOM	2156	CB	TYR	B	700	17.611	24.657	38.322	1.00	32.62	C
ATOM	2157	CG	TYR	B	700	16.777	25.425	39.335	1.00	36.19	C
ATOM	2158	CD1	TYR	B	700	16.805	24.932	40.651	1.00	37.04	CD2 C
ATOM	2159	CD2	TYR	B	700	15.981	26.546	39.017	1.00	36.03	CD1 C
ATOM	2160	CE1	TYR	B	700	16.094	25.561	41.660	1.00	37.50	CE2 C
ATOM	2161	CE2	TYR	B	700	15.258	27.174	40.020	1.00	37.46	CE1 C
ATOM	2162	CZ	TYR	B	700	15.322	26.667	41.320	1.00	39.74	C
ATOM	2163	OH	TYR	B	700	14.692	27.178	42.459	1.00	42.32	O
ATOM	2164	N	ALA	B	701	17.349	23.495	35.462	1.00	35.50	N
ATOM	2165	CA	ALA	B	701	18.218	23.230	34.333	1.00	37.81	C
ATOM	2166	C	ALA	B	701	19.615	23.862	34.435	1.00	40.25	C
ATOM	2167	O	ALA	B	701	20.526	23.374	33.719	1.00	38.61	O
ATOM	2168	CB	ALA	B	701	17.505	23.664	33.039	1.00	33.57	C
ATOM	2169	N	GLY	B	702	19.869	24.905	35.225	1.00	42.37	N
ATOM	2170	CA	GLY	B	702	20.990	25.773	35.026	1.00	49.04	C
ATOM	2171	C	GLY	B	702	21.179	26.585	33.768	1.00	54.21	C
ATOM	2172	O	GLY	B	702	22.308	26.900	33.378	1.00	54.06	O
ATOM	2173	N	HIS	B	703	20.147	27.025	33.051	1.00	59.42	N
ATOM	2174	CA	HIS	B	703	20.150	27.368	31.633	1.00	63.18	C
ATOM	2175	C	HIS	B	703	20.270	28.869	31.342	1.00	67.64	C
ATOM	2176	O	HIS	B	703	19.717	29.666	32.133	1.00	68.78	O
ATOM	2177	CB	HIS	B	703	18.858	26.944	30.950	1.00	61.19	C

FIG. 7 CONT'D

ATOM	2178	CG	HIS	B	703	18.704	27.489	29.562	1.00	60.45	C
ATOM	2179	ND1	HIS	B	703	18.060	28.667	29.318	1.00	59.69	N
ATOM	2180	CD2	HIS	B	703	19.138	27.007	28.378	1.00	60.07	C
ATOM	2181	CE1	HIS	B	703	18.085	28.834	27.998	1.00	60.73	C
ATOM	2182	NE2	HIS	B	703	18.724	27.840	27.394	1.00	59.97	N
ATOM	2183	N	ASP	B	704	20.844	29.266	30.169	1.00	71.63	N
ATOM	2184	CA	ASP	B	704	21.362	30.640	30.148	1.00	74.67	C
ATOM	2185	C	ASP	B	704	20.165	31.589	30.240	1.00	76.34	C
ATOM	2186	O	ASP	B	704	20.278	32.495	31.089	1.00	78.77	O
ATOM	2187	CB	ASP	B	704	22.338	31.126	29.089	1.00	74.21	C
ATOM	2188	CG	ASP	B	704	23.262	32.333	29.288	1.00	72.26	C
ATOM	2189	OD1	ASP	B	704	23.532	32.982	30.339	1.00	69.97	O
ATOM	2190	OD2	ASP	B	704	23.880	32.743	28.267	1.00	70.10	O
ATOM	2191	N	ASN	B	705	19.178	31.536	29.392	1.00	76.44	N
ATOM	2192	CA	ASN	B	705	18.121	32.537	29.376	1.00	77.88	C
ATOM	2193	C	ASN	B	705	18.552	33.977	29.159	1.00	78.69	C
ATOM	2194	O	ASN	B	705	17.600	34.732	28.837	1.00	80.54	O
ATOM	2195	CB	ASN	B	705	17.167	32.382	30.579	1.00	77.36	C
ATOM	2196	CG	ASN	B	705	15.975	31.486	30.276	1.00	76.69	C
ATOM	2197	OD1	ASN	B	705	15.403	31.587	29.187	1.00	75.75	O
ATOM	2198	ND2	ASN	B	705	15.561	30.578	31.149	1.00	75.65	N
ATOM	2199	N	THR	B	706	19.783	34.455	29.193	1.00	78.32	N
ATOM	2200	CA	THR	B	706	20.093	35.733	28.559	1.00	78.30	C
ATOM	2201	C	THR	B	706	20.205	35.454	27.059	1.00	80.20	C
ATOM	2202	O	THR	B	706	19.535	36.020	26.181	1.00	81.40	O
ATOM	2203	CB	THR	B	706	21.334	36.419	29.139	1.00	76.92	C
ATOM	2204	OG1	THR	B	706	22.521	35.748	28.718	1.00	75.69	O
ATOM	2205	CG2	THR	B	706	21.210	36.466	30.660	1.00	75.77	C
ATOM	2206	N	LYS	B	707	20.997	34.411	26.758	1.00	80.80	N
ATOM	2207	CA	LYS	B	707	21.296	34.137	25.348	1.00	79.77	C
ATOM	2208	C	LYS	B	707	19.977	34.028	24.602	1.00	78.58	C
ATOM	2209	O	LYS	B	707	18.894	33.829	25.149	1.00	77.58	O
ATOM	2210	CB	LYS	B	707	22.192	32.910	25.210	1.00	80.10	C
ATOM	2211	CG	LYS	B	707	23.693	33.111	25.185	1.00	80.02	C
ATOM	2212	CD	LYS	B	707	24.330	33.085	23.807	1.00	80.70	C
ATOM	2213	CE	LYS	B	707	25.492	34.048	23.655	1.00	80.79	C
ATOM	2214	NZ	LYS	B	707	26.610	33.537	22.817	1.00	80.22	N
ATOM	2215	N	PRO	B	708	20.110	34.208	23.287	1.00	79.44	N
ATOM	2216	CA	PRO	B	708	19.079	33.723	22.388	1.00	78.75	C
ATOM	2217	C	PRO	B	708	19.191	32.250	22.035	1.00	77.52	C
ATOM	2218	O	PRO	B	708	20.140	31.862	21.349	1.00	77.23	O
ATOM	2219	CB	PRO	B	708	19.249	34.560	21.139	1.00	79.21	C
ATOM	2220	CG	PRO	B	708	20.215	35.642	21.431	1.00	79.73	C
ATOM	2221	CD	PRO	B	708	20.897	35.351	22.732	1.00	79.25	C
ATOM	2222	N	ASP	B	709	18.207	31.458	22.451	1.00	75.85	N
ATOM	2223	CA	ASP	B	709	18.130	30.016	22.275	1.00	73.49	C
ATOM	2224	C	ASP	B	709	18.757	29.547	20.968	1.00	70.98	C
ATOM	2225	O	ASP	B	709	18.267	30.048	19.960	1.00	72.76	O
ATOM	2226	CB	ASP	B	709	16.708	29.501	22.165	1.00	72.50	C
ATOM	2227	CG	ASP	B	709	15.686	29.263	23.200	1.00	72.04	C
ATOM	2228	OD1	ASP	B	709	15.852	28.797	24.336	1.00	72.35	O
ATOM	2229	OD2	ASP	B	709	14.497	29.544	22.898	1.00	72.06	O
ATOM	2230	N	THR	B	710	19.721	28.667	20.914	1.00	66.40	N
ATOM	2231	CA	THR	B	710	20.014	27.973	19.647	1.00	61.30	C
ATOM	2232	C	THR	B	710	19.461	26.568	19.771	1.00	58.36	C
ATOM	2233	O	THR	B	710	19.043	26.179	20.867	1.00	55.98	O
ATOM	2234	CB	THR	B	710	21.508	28.082	19.347	1.00	60.69	C
ATOM	2235	OG1	THR	B	710	22.295	27.394	20.327	1.00	60.91	O
ATOM	2236	CG2	THR	B	710	22.080	29.499	19.448	1.00	59.72	C
ATOM	2237	N	SER	B	711	19.372	25.757	18.731	1.00	56.41	N
ATOM	2238	CA	SER	B	711	18.604	24.501	18.872	1.00	54.86	C
ATOM	2239	C	SER	B	711	19.459	23.523	19.689	1.00	53.52	C
ATOM	2240	O	SER	B	711	19.064	22.792	20.602	1.00	53.19	O
ATOM	2241	CB	SER	B	711	18.136	23.866	17.576	1.00	54.22	C

FIG. 7 CONT'D

ATOM	2242	OG	SER	B	711	19.016	22.895	17.016	1.00	55.08	O
ATOM	2243	N	SER	B	712	20.762	23.540	19.438	1.00	50.94	N
ATOM	2244	CA	SER	B	712	21.602	22.647	20.202	1.00	48.78	C
ATOM	2245	C	SER	B	712	21.719	23.090	21.650	1.00	47.52	C
ATOM	2246	O	SER	B	712	21.962	22.224	22.506	1.00	48.28	O
ATOM	2247	CB	SER	B	712	22.987	22.575	19.568	1.00	49.25	C
ATOM	2248	OG	SER	B	712	23.464	23.918	19.761	1.00	49.47	O
ATOM	2249	N	SER	B	713	21.571	24.368	21.976	1.00	43.60	N
ATOM	2250	CA	SER	B	713	21.831	24.897	23.308	1.00	37.97	C
ATOM	2251	C	SER	B	713	20.656	24.477	24.153	1.00	33.45	C
ATOM	2252	O	SER	B	713	20.789	24.032	25.260	1.00	30.49	O
ATOM	2253	CB	SER	B	713	22.119	26.420	23.343	1.00	35.58	C
ATOM	2254	OG	SER	B	713	21.049	27.201	23.849	1.00	33.18	O
ATOM	2255	N	LEU	B	714	19.463	24.645	23.672	1.00	30.82	N
ATOM	2256	CA	LEU	B	714	18.252	24.084	24.240	1.00	30.72	C
ATOM	2257	C	LEU	B	714	18.345	22.574	24.502	1.00	29.98	C
ATOM	2258	O	LEU	B	714	18.048	22.146	25.613	1.00	28.50	O
ATOM	2259	CB	LEU	B	714	16.982	24.360	23.369	1.00	29.76	C
ATOM	2260	CG	LEU	B	714	15.672	24.165	24.162	1.00	28.05	C
ATOM	2261	CD1	LEU	B	714	15.444	25.280	25.180	1.00	24.17	C
ATOM	2262	CD2	LEU	B	714	14.501	23.972	23.219	1.00	25.57	C
ATOM	2263	N	LEU	B	715	18.773	21.817	23.489	1.00	27.99	N
ATOM	2264	CA	LEU	B	715	18.862	20.392	23.591	1.00	24.13	C
ATOM	2265	C	LEU	B	715	19.950	20.032	24.598	1.00	25.10	C
ATOM	2266	O	LEU	B	715	19.701	19.146	25.446	1.00	25.65	O
ATOM	2267	CB	LEU	B	715	19.038	19.679	22.268	1.00	17.53	C
ATOM	2268	CG	LEU	B	715	17.953	19.716	21.238	1.00	9.68	C
ATOM	2269	CD1	LEU	B	715	18.617	19.353	19.949	1.00	10.52	C
ATOM	2270	CD2	LEU	B	715	16.695	18.930	21.494	1.00	2.63	C
ATOM	2271	N	THR	B	716	21.090	20.669	24.467	1.00	24.67	N
ATOM	2272	CA	THR	B	716	22.073	20.564	25.560	1.00	25.89	C
ATOM	2273	C	THR	B	716	21.650	21.015	26.943	1.00	25.65	C
ATOM	2274	O	THR	B	716	22.242	20.528	27.888	1.00	28.59	O
ATOM	2275	CB	THR	B	716	23.357	21.293	25.092	1.00	24.06	C
ATOM	2276	OG1	THR	B	716	23.941	20.511	24.053	1.00	23.61	O
ATOM	2277	CG2	THR	B	716	24.220	21.618	26.290	1.00	21.80	C
ATOM	2278	N	SER	B	717	20.702	21.817	27.263	1.00	25.76	N
ATOM	2279	CA	SER	B	717	20.187	22.202	28.524	1.00	25.78	C
ATOM	2280	C	SER	B	717	19.225	21.188	29.075	1.00	24.82	C
ATOM	2281	O	SER	B	717	19.269	20.792	30.216	1.00	23.76	O
ATOM	2282	CB	SER	B	717	19.385	23.513	28.238	1.00	26.46	C
ATOM	2283	OG	SER	B	717	20.363	24.508	27.930	1.00	28.06	O
ATOM	2284	N	LEU	B	718	18.359	20.753	28.151	1.00	24.39	N
ATOM	2285	CA	LEU	B	718	17.459	19.628	28.373	1.00	24.32	C
ATOM	2286	C	LEU	B	718	18.166	18.389	28.954	1.00	25.41	C
ATOM	2287	O	LEU	B	718	17.676	17.715	29.870	1.00	26.08	O
ATOM	2288	CB	LEU	B	718	16.533	19.275	27.180	1.00	20.51	C
ATOM	2289	CG	LEU	B	718	15.238	20.105	27.051	1.00	17.72	C
ATOM	2290	CD1	LEU	B	718	14.657	19.712	25.707	1.00	16.34	C
ATOM	2291	CD2	LEU	B	718	14.194	20.017	28.125	1.00	15.03	C
ATOM	2292	N	ASN	B	719	19.344	18.031	28.458	1.00	23.01	N
ATOM	2293	CA	ASN	B	719	20.019	16.841	28.870	1.00	18.99	C
ATOM	2294	C	ASN	B	719	20.534	17.050	30.258	1.00	20.15	C
ATOM	2295	O	ASN	B	719	20.168	16.370	31.195	1.00	20.10	O
ATOM	2296	CB	ASN	B	719	21.155	16.550	27.924	1.00	17.32	C
ATOM	2297	CG	ASN	B	719	20.791	15.956	26.547	1.00	14.40	C
ATOM	2298	OD1	ASN	B	719	19.658	15.685	26.080	1.00	10.28	O
ATOM	2299	ND2	ASN	B	719	22.009	15.736	25.997	1.00	10.72	N
ATOM	2300	N	GLN	B	720	21.372	18.084	30.313	1.00	20.82	N
ATOM	2301	CA	GLN	B	720	21.748	18.648	31.620	1.00	18.86	C
ATOM	2302	C	GLN	B	720	20.638	18.425	32.648	1.00	20.04	C
ATOM	2303	O	GLN	B	720	20.727	17.588	33.537	1.00	14.79	O
ATOM	2304	CB	GLN	B	720	22.086	20.115	31.433	1.00	16.30	C
ATOM	2305	CG	GLN	B	720	22.684	20.561	32.806	1.00	22.15	C

FIG. 7 CONT'D

ATOM	2306	CD	GLN	B	720	24.065	21.100	32.473	1.00	26.00	C
ATOM	2307	OE1	GLN	B	720	24.479	20.724	31.344	1.00	29.16	O
ATOM	2308	NE2	GLN	B	720	24.788	21.874	33.272	1.00	25.14	N
ATOM	2309	N	LEU	B	721	19.498	19.161	32.465	1.00	21.93	N
ATOM	2310	CA	LEU	B	721	18.382	18.967	33.385	1.00	19.17	C
ATOM	2311	C	LEU	B	721	18.045	17.470	33.471	1.00	19.89	C
ATOM	2312	O	LEU	B	721	17.735	17.027	34.576	1.00	15.63	O
ATOM	2313	CB	LEU	B	721	17.191	19.813	33.060	1.00	15.39	C
ATOM	2314	CG	LEU	B	721	15.760	19.424	33.469	1.00	15.22	C
ATOM	2315	CD1	LEU	B	721	15.669	19.501	34.979	1.00	13.96	C
ATOM	2316	CD2	LEU	B	721	14.618	20.136	32.748	1.00	10.16	C
ATOM	2317	N	GLY	B	722	18.053	16.691	32.388	1.00	19.37	N
ATOM	2318	CA	GLY	B	722	17.897	15.291	32.388	1.00	21.33	C
ATOM	2319	C	GLY	B	722	18.758	14.464	33.309	1.00	23.40	C
ATOM	2320	O	GLY	B	722	18.285	13.747	34.197	1.00	23.39	O
ATOM	2321	N	GLU	B	723	20.057	14.691	33.176	1.00	21.76	N
ATOM	2322	CA	GLU	B	723	21.026	14.136	34.156	1.00	19.33	C
ATOM	2323	C	GLU	B	723	20.568	14.373	35.563	1.00	22.18	C
ATOM	2324	O	GLU	B	723	20.464	13.450	36.403	1.00	22.37	O
ATOM	2325	CB	GLU	B	723	22.333	14.720	33.711	1.00	15.68	C
ATOM	2326	CG	GLU	B	723	23.578	14.510	34.542	1.00	13.79	C
ATOM	2327	CD	GLU	B	723	23.977	13.134	34.198	1.00	14.42	C
ATOM	2328	OE1	GLU	B	723	23.157	12.555	33.447	1.00	14.44	O
ATOM	2329	OE2	GLU	B	723	24.947	12.470	34.526	1.00	15.17	O
ATOM	2330	N	ARG	B	724	20.128	15.611	35.902	1.00	24.67	N
ATOM	2331	CA	ARG	B	724	19.831	16.036	37.268	1.00	23.49	C
ATOM	2332	C	ARG	B	724	18.572	15.318	37.733	1.00	23.59	C
ATOM	2333	O	ARG	B	724	18.370	14.910	38.864	1.00	24.14	O
ATOM	2334	CB	ARG	B	724	19.720	17.533	37.453	1.00	21.12	C
ATOM	2335	CG	ARG	B	724	21.059	18.178	37.063	1.00	21.15	C
ATOM	2336	CD	ARG	B	724	20.863	19.621	37.339	1.00	26.14	C
ATOM	2337	NE	ARG	B	724	21.327	20.657	36.494	1.00	29.20	N
ATOM	2338	CZ	ARG	B	724	22.167	21.650	36.526	1.00	27.46	C
ATOM	2339	NH1	ARG	B	724	22.925	22.020	37.503	1.00	25.52	N
ATOM	2340	NH2	ARG	B	724	22.186	22.354	35.404	1.00	29.60	N
ATOM	2341	N	GLN	B	725	17.775	14.904	36.775	1.00	23.33	N
ATOM	2342	CA	GLN	B	725	16.526	14.265	37.177	1.00	22.49	C
ATOM	2343	C	GLN	B	725	16.753	12.805	37.497	1.00	22.21	C
ATOM	2344	O	GLN	B	725	16.048	12.218	38.307	1.00	24.21	O
ATOM	2345	CB	GLN	B	725	15.530	14.650	36.092	1.00	19.78	C
ATOM	2346	CG	GLN	B	725	14.973	16.030	36.372	1.00	18.29	C
ATOM	2347	CD	GLN	B	725	13.791	16.367	35.521	1.00	20.58	C
ATOM	2348	OE1	GLN	B	725	13.122	15.365	35.166	1.00	20.92	O
ATOM	2349	NE2	GLN	B	725	13.530	17.685	35.215	1.00	20.42	N
ATOM	2350	N	LEU	B	726	17.725	12.161	36.890	1.00	18.53	N
ATOM	2351	CA	LEU	B	726	17.939	10.728	36.974	1.00	11.85	C
ATOM	2352	C	LEU	B	726	18.596	10.516	38.325	1.00	13.48	C
ATOM	2353	O	LEU	B	726	18.344	9.605	39.078	1.00	5.74	O
ATOM	2354	CB	LEU	B	726	19.079	10.330	36.078	1.00	2.80	C
ATOM	2355	CG	LEU	B	726	19.502	9.112	35.317	1.00	5.40	C
ATOM	2356	CD1	LEU	B	726	18.241	8.231	35.093	1.00	4.71	C
ATOM	2357	CD2	LEU	B	726	20.096	9.582	33.987	1.00	2.67	C
ATOM	2358	N	LEU	B	727	19.607	11.399	38.614	1.00	16.72	N
ATOM	2359	CA	LEU	B	727	20.057	11.420	40.026	1.00	18.66	C
ATOM	2360	C	LEU	B	727	18.888	11.591	40.971	1.00	21.90	C
ATOM	2361	O	LEU	B	727	18.636	10.857	41.927	1.00	23.67	O
ATOM	2362	CB	LEU	B	727	21.072	12.497	39.953	1.00	15.99	C
ATOM	2363	CG	LEU	B	727	22.514	12.219	39.641	1.00	15.34	C
ATOM	2364	CD1	LEU	B	727	23.203	13.523	40.096	1.00	17.49	C
ATOM	2365	CD2	LEU	B	727	23.106	11.066	40.427	1.00	12.70	C
ATOM	2366	N	SER	B	728	17.975	12.544	40.742	1.00	21.04	N
ATOM	2367	CA	SER	B	728	16.751	12.597	41.511	1.00	19.14	C
ATOM	2368	C	SER	B	728	15.931	11.322	41.639	1.00	16.91	C
ATOM	2369	O	SER	B	728	15.370	11.088	42.680	1.00	13.08	O

FIG. 7 CONT'D

ATOM	2370	CB	SER	B	728	15.848	13.675	40.896	1.00	21.55	C
ATOM	2371	OG	SER	B	728	15.135	14.366	41.938	1.00	22.86	O
ATOM	2372	N	VAL	B	729	15.749	10.596	40.531	1.00	15.00	N
ATOM	2373	CA	VAL	B	729	15.173	9.282	40.490	1.00	12.17	C
ATOM	2374	C	VAL	B	729	15.879	8.202	41.323	1.00	10.68	C
ATOM	2375	O	VAL	B	729	15.231	7.392	41.943	1.00	2.48	O
ATOM	2376	CB	VAL	B	729	15.178	8.766	39.037	1.00	10.15	C
ATOM	2377	CG1	VAL	B	729	14.487	7.448	38.770	1.00	2.02	C
ATOM	2378	CG2	VAL	B	729	14.330	9.852	38.390	1.00	10.13	C
ATOM	2379	N	VAL	B	730	17.202	8.146	41.316	1.00	2.02	N
ATOM	2380	CA	VAL	B	730	17.862	7.116	42.020	1.00	10.25	C
ATOM	2381	C	VAL	B	730	17.621	7.319	43.484	1.00	16.17	C
ATOM	2382	O	VAL	B	730	17.157	6.467	44.259	1.00	16.44	O
ATOM	2383	CB	VAL	B	730	19.310	7.130	41.578	1.00	7.06	C
ATOM	2384	CG1	VAL	B	730	20.320	6.553	42.490	1.00	5.61	C
ATOM	2385	CG2	VAL	B	730	19.298	6.450	40.221	1.00	8.10	C
ATOM	2386	N	LYS	B	731	17.795	8.560	43.943	1.00	22.22	N
ATOM	2387	CA	LYS	B	731	17.657	8.834	45.372	1.00	23.44	C
ATOM	2388	C	LYS	B	731	16.165	8.661	45.673	1.00	22.32	C
ATOM	2389	O	LYS	B	731	15.880	8.168	46.791	1.00	22.54	O
ATOM	2390	CB	LYS	B	731	18.323	10.151	45.666	1.00	25.76	C
ATOM	2391	CG	LYS	B	731	17.637	11.081	46.669	1.00	25.80	C
ATOM	2392	CD	LYS	B	731	18.665	11.681	47.571	1.00	30.65	C
ATOM	2393	CE	LYS	B	731	19.117	11.123	48.913	1.00	28.19	C
ATOM	2394	NZ	LYS	B	731	19.670	12.349	49.663	1.00	25.43	N
ATOM	2395	N	TRP	B	732	15.288	8.938	44.720	1.00	17.22	N
ATOM	2396	CA	TRP	B	732	13.921	8.754	45.123	1.00	15.59	C
ATOM	2397	C	TRP	B	732	13.631	7.299	45.344	1.00	14.62	C
ATOM	2398	O	TRP	B	732	13.079	6.898	46.346	1.00	12.62	O
ATOM	2399	CB	TRP	B	732	13.048	9.440	44.110	1.00	13.17	C
ATOM	2400	CG	TRP	B	732	11.590	9.146	44.070	1.00	9.03	C
ATOM	2401	CD1	TRP	B	732	10.630	9.636	44.895	1.00	6.61	C
ATOM	2402	CD2	TRP	B	732	10.943	8.272	43.129	1.00	7.56	C
ATOM	2403	NE1	TRP	B	732	9.393	9.151	44.548	1.00	6.61	N
ATOM	2404	CE2	TRP	B	732	9.567	8.315	43.447	1.00	6.62	C
ATOM	2405	CE3	TRP	B	732	11.378	7.470	42.076	1.00	6.83	C
ATOM	2406	CZ2	TRP	B	732	8.623	7.567	42.729	1.00	2.95	C
ATOM	2407	CZ3	TRP	B	732	10.362	6.743	41.384	1.00	6.78	C
ATOM	2408	CH2	TRP	B	732	8.993	6.762	41.721	1.00	3.62	C
ATOM	2409	N	SER	B	733	13.995	6.411	44.459	1.00	16.43	N
ATOM	2410	CA	SER	B	733	13.755	4.957	44.528	1.00	16.59	C
ATOM	2411	C	SER	B	733	14.360	4.325	45.815	1.00	15.61	C
ATOM	2412	O	SER	B	733	13.643	3.450	46.377	1.00	4.55	O
ATOM	2413	CB	SER	B	733	14.232	4.096	43.348	1.00	12.94	C
ATOM	2414	OG	SER	B	733	15.556	4.363	42.917	1.00	8.63	O
ATOM	2415	N	LYS	B	734	15.507	4.879	46.229	1.00	14.78	N
ATOM	2416	CA	LYS	B	734	16.148	4.475	47.448	1.00	17.27	C
ATOM	2417	C	LYS	B	734	15.282	4.700	48.666	1.00	17.41	C
ATOM	2418	O	LYS	B	734	15.513	3.908	49.597	1.00	16.69	O
ATOM	2419	CB	LYS	B	734	17.613	4.984	47.566	1.00	16.61	C
ATOM	2420	CG	LYS	B	734	18.658	4.251	46.834	1.00	17.18	C
ATOM	2421	CD	LYS	B	734	20.025	3.972	46.428	1.00	17.70	C
ATOM	2422	CE	LYS	B	734	20.895	5.215	46.518	1.00	22.56	C
ATOM	2423	NZ	LYS	B	734	22.295	5.017	47.121	1.00	22.89	N
ATOM	2424	N	SER	B	735	14.275	5.551	48.728	1.00	15.13	N
ATOM	2425	CA	SER	B	735	13.218	5.538	49.674	1.00	12.68	C
ATOM	2426	C	SER	B	735	11.833	5.075	49.321	1.00	14.41	C
ATOM	2427	O	SER	B	735	11.004	5.265	50.204	1.00	13.41	O
ATOM	2428	CB	SER	B	735	12.793	6.975	49.834	1.00	11.81	C
ATOM	2429	OG	SER	B	735	13.355	7.718	50.772	1.00	12.00	O
ATOM	2430	N	LEU	B	736	11.487	4.753	48.094	1.00	15.17	N
ATOM	2431	CA	LEU	B	736	10.229	4.063	47.787	1.00	17.13	C
ATOM	2432	C	LEU	B	736	10.055	2.709	48.516	1.00	20.03	C
ATOM	2433	O	LEU	B	736	10.985	1.886	48.636	1.00	20.04	O

FIG. 7 CONT'D

ATOM	2434	CB	LEU	B	736	10.227	3.715	46.291	1.00	13.29	C
ATOM	2435	CG	LEU	B	736	8.963	3.411	45.495	1.00	8.90	C
ATOM	2436	CD1	LEU	B	736	7.760	4.198	45.906	1.00	2.02	C
ATOM	2437	CD2	LEU	B	736	9.292	3.404	43.989	1.00	6.33	C
ATOM	2438	N	PRO	B	737	8.915	2.608	49.200	1.00	18.86	N
ATOM	2439	CA	PRO	B	737	8.660	1.437	50.012	1.00	16.10	C
ATOM	2440	C	PRO	B	737	8.564	0.201	49.149	1.00	15.61	C
ATOM	2441	O	PRO	B	737	7.766	0.190	48.217	1.00	20.02	O
ATOM	2442	CB	PRO	B	737	7.584	1.910	50.961	1.00	9.40	C
ATOM	2443	CG	PRO	B	737	6.981	3.068	50.335	1.00	13.50	C
ATOM	2444	CD	PRO	B	737	8.051	3.785	49.539	1.00	15.00	C
ATOM	2445	N	GLY	B	738	9.452	-0.776	49.166	1.00	15.25	N
ATOM	2446	CA	GLY	B	738	9.507	-1.955	48.327	1.00	15.32	C
ATOM	2447	C	GLY	B	738	10.696	-1.873	47.426	1.00	18.15	C
ATOM	2448	O	GLY	B	738	11.399	-2.857	47.387	1.00	20.68	O
ATOM	2449	N	PHE	B	739	11.005	-0.740	46.754	1.00	18.75	N
ATOM	2450	CA	PHE	B	739	12.006	-0.790	45.700	1.00	17.86	C
ATOM	2451	C	PHE	B	739	13.298	-1.465	46.088	1.00	17.65	C
ATOM	2452	O	PHE	B	739	13.808	-2.367	45.389	1.00	16.39	O
ATOM	2453	CB	PHE	B	739	12.211	0.503	44.967	1.00	15.09	C
ATOM	2454	CG	PHE	B	739	12.706	0.335	43.543	1.00	12.77	C
ATOM	2455	CD1	PHE	B	739	12.021	-0.479	42.643	1.00	12.86	C
ATOM	2456	CD2	PHE	B	739	13.853	0.972	43.162	1.00	9.22	C
ATOM	2457	CE1	PHE	B	739	12.545	-0.636	41.356	1.00	14.77	C
ATOM	2458	CE2	PHE	B	739	14.376	0.860	41.923	1.00	10.28	C
ATOM	2459	CZ	PHE	B	739	13.717	0.058	41.020	1.00	14.00	C
ATOM	2460	N	ARG	B	740	13.711	-1.458	47.358	1.00	19.11	N
ATOM	2461	CA	ARG	B	740	15.080	-1.785	47.677	1.00	19.58	C
ATOM	2462	C	ARG	B	740	15.162	-3.226	48.076	1.00	21.62	C
ATOM	2463	O	ARG	B	740	16.237	-3.661	48.234	1.00	21.22	O
ATOM	2464	CB	ARG	B	740	15.590	-0.970	48.833	1.00	14.39	C
ATOM	2465	CG	ARG	B	740	14.456	-1.061	49.873	1.00	11.17	C
ATOM	2466	CD	ARG	B	740	15.098	-0.835	51.207	1.00	2.02	C
ATOM	2467	NE	ARG	B	740	14.276	-0.848	52.359	1.00	2.27	N
ATOM	2468	CZ	ARG	B	740	14.684	-0.546	53.553	1.00	5.35	C
ATOM	2469	NH1	ARG	B	740	15.938	-0.149	53.779	1.00	3.17	N
ATOM	2470	NH2	ARG	B	740	13.718	-0.591	54.446	1.00	5.71	N
ATOM	2471	N	ASN	B	741	14.054	-3.896	48.128	1.00	25.22	N
ATOM	2472	CA	ASN	B	741	13.950	-5.346	48.309	1.00	24.57	C
ATOM	2473	C	ASN	B	741	13.976	-6.071	46.978	1.00	24.79	C
ATOM	2474	O	ASN	B	741	14.081	-7.316	47.038	1.00	25.54	O
ATOM	2475	CB	ASN	B	741	12.644	-5.611	49.138	1.00	21.04	C
ATOM	2476	CG	ASN	B	741	12.858	-4.759	50.433	1.00	20.92	C
ATOM	2477	OD1	ASN	B	741	11.844	-4.356	50.998	1.00	18.35	O
ATOM	2478	ND2	ASN	B	741	14.035	-4.413	50.985	1.00	15.77	N
ATOM	2479	N	LEU	B	742	13.932	-5.378	45.841	1.00	24.61	N
ATOM	2480	CA	LEU	B	742	14.347	-6.030	44.616	1.00	22.66	C
ATOM	2481	C	LEU	B	742	15.805	-6.252	44.450	1.00	21.69	C
ATOM	2482	O	LEU	B	742	16.521	-5.399	44.847	1.00	17.38	O
ATOM	2483	CB	LEU	B	742	14.036	-5.110	43.412	1.00	23.20	C
ATOM	2484	CG	LEU	B	742	12.533	-4.825	43.313	1.00	22.70	C
ATOM	2485	CD1	LEU	B	742	12.226	-4.297	41.935	1.00	20.93	C
ATOM	2486	CD2	LEU	B	742	11.722	-6.084	43.665	1.00	20.75	C
ATOM	2487	N	HIS	B	743	16.221	-7.275	43.773	1.00	25.36	N
ATOM	2488	CA	HIS	B	743	17.606	-7.471	43.441	1.00	29.42	C
ATOM	2489	C	HIS	B	743	18.270	-6.197	42.971	1.00	29.20	C
ATOM	2490	O	HIS	B	743	17.656	-5.654	42.078	1.00	31.07	O
ATOM	2491	CB	HIS	B	743	17.688	-8.560	42.354	1.00	29.50	C
ATOM	2492	CG	HIS	B	743	19.140	-9.002	42.332	1.00	32.72	C
ATOM	2493	ND1	HIS	B	743	20.151	-8.126	41.921	1.00	33.59	N
ATOM	2494	CD2	HIS	B	743	19.719	-10.158	42.717	1.00	31.20	C
ATOM	2495	CE1	HIS	B	743	21.290	-8.773	42.069	1.00	34.00	C
ATOM	2496	NE2	HIS	B	743	21.057	-9.993	42.505	1.00	32.06	N
ATOM	2497	N	ILE	B	744	19.483	-5.832	43.276	1.00	27.47	N

FIG. 7 CONT'D

ATOM	2498	CA	ILE	B	744	20.179	-4.660	42.787	1.00	26.82	C
ATOM	2499	C	ILE	B	744	19.943	-4.370	41.316	1.00	27.24	C
ATOM	2500	O	ILE	B	744	19.667	-3.217	40.917	1.00	25.94	O
ATOM	2501	CB	ILE	B	744	21.681	-4.720	43.182	1.00	22.87	C
ATOM	2502	CG1	ILE	B	744	22.187	-3.390	43.708	1.00	18.55	C
ATOM	2503	CG2	ILE	B	744	22.664	-5.241	42.146	1.00	20.70	C
ATOM	2504	CD1	ILE	B	744	22.455	-2.206	42.845	1.00	19.16	C
ATOM	2505	N	ASP	B	745	20.125	-5.399	40.512	1.00	27.64	N
ATOM	2506	CA	ASP	B	745	20.178	-5.411	39.059	1.00	26.39	C
ATOM	2507	C	ASP	B	745	18.914	-5.043	38.375	1.00	23.52	C
ATOM	2508	O	ASP	B	745	18.949	-4.407	37.397	1.00	22.77	O
ATOM	2509	CB	ASP	B	745	20.569	-6.913	38.930	1.00	28.78	C
ATOM	2510	CG	ASP	B	745	22.050	-6.940	38.594	1.00	30.56	C
ATOM	2511	OD1	ASP	B	745	22.523	-5.759	38.461	1.00	33.10	O
ATOM	2512	OD2	ASP	B	745	22.613	-8.025	38.424	1.00	28.71	O
ATOM	2513	N	ASP	B	746	17.791	-5.485	38.861	1.00	20.37	N
ATOM	2514	CA	ASP	B	746	16.461	-5.254	38.523	1.00	19.80	C
ATOM	2515	C	ASP	B	746	16.101	-3.849	38.838	1.00	21.17	C
ATOM	2516	O	ASP	B	746	15.426	-3.133	38.104	1.00	23.20	O
ATOM	2517	CB	ASP	B	746	15.525	-6.172	39.278	1.00	17.56	C
ATOM	2518	CG	ASP	B	746	15.697	-7.662	38.927	1.00	18.00	C
ATOM	2519	OD1	ASP	B	746	16.060	-8.029	37.734	1.00	17.86	O
ATOM	2520	OD2	ASP	B	746	15.399	-8.360	39.945	1.00	10.81	O
ATOM	2521	N	GLN	B	747	16.381	-3.300	39.971	1.00	21.37	N
ATOM	2522	CA	GLN	B	747	16.235	-1.870	40.231	1.00	19.26	C
ATOM	2523	C	GLN	B	747	17.113	-1.028	39.295	1.00	19.78	C
ATOM	2524	O	GLN	B	747	16.684	0.096	39.085	1.00	19.77	O
ATOM	2525	CB	GLN	B	747	16.565	-1.553	41.691	1.00	17.84	C
ATOM	2526	CG	GLN	B	747	16.011	-2.086	42.961	1.00	13.39	C
ATOM	2527	CD	GLN	B	747	16.788	-2.064	44.276	1.00	11.14	C
ATOM	2528	OE1	GLN	B	747	17.279	-1.032	44.749	1.00	13.14	O
ATOM	2529	NE2	GLN	B	747	16.992	-3.141	45.001	1.00	6.87	N
ATOM	2530	N	ILE	B	748	18.321	-1.447	38.878	1.00	18.38	N
ATOM	2531	CA	ILE	B	748	18.953	-0.798	37.751	1.00	17.05	C
ATOM	2532	C	ILE	B	748	18.215	-1.041	36.455	1.00	17.46	C
ATOM	2533	O	ILE	B	748	17.992	-0.001	35.886	1.00	20.47	O
ATOM	2534	CB	ILE	B	748	20.424	-1.069	37.413	1.00	13.20	C
ATOM	2535	CG1	ILE	B	748	21.184	-0.786	38.681	1.00	12.04	C
ATOM	2536	CG2	ILE	B	748	20.763	-0.264	36.156	1.00	7.66	C
ATOM	2537	CD1	ILE	B	748	21.757	-1.682	39.692	1.00	8.58	C
ATOM	2538	N	THR	B	749	17.809	-2.196	36.013	1.00	16.06	N
ATOM	2539	CA	THR	B	749	16.934	-2.329	34.878	1.00	14.15	C
ATOM	2540	C	THR	B	749	15.678	-1.460	34.916	1.00	15.06	C
ATOM	2541	O	THR	B	749	15.407	-0.806	33.894	1.00	13.33	O
ATOM	2542	CB	THR	B	749	16.782	-3.841	34.569	1.00	11.27	C
ATOM	2543	OG1	THR	B	749	18.137	-4.238	34.410	1.00	10.00	O
ATOM	2544	CG2	THR	B	749	16.199	-4.144	33.198	1.00	8.36	C
ATOM	2545	N	LEU	B	750	14.901	-1.431	35.998	1.00	14.67	N
ATOM	2546	CA	LEU	B	750	13.667	-0.653	35.984	1.00	11.74	C
ATOM	2547	C	LEU	B	750	13.848	0.856	36.005	1.00	11.04	C
ATOM	2548	O	LEU	B	750	13.174	1.592	35.266	1.00	10.56	O
ATOM	2549	CB	LEU	B	750	12.690	-1.020	37.085	1.00	7.25	C
ATOM	2550	CG	LEU	B	750	12.542	-2.574	37.194	1.00	3.91	C
ATOM	2551	CD1	LEU	B	750	12.329	-2.847	38.676	1.00	2.28	C
ATOM	2552	CD2	LEU	B	750	11.463	-2.846	36.206	1.00	2.86	C
ATOM	2553	N	ILE	B	751	14.940	1.269	36.654	1.00	9.75	N
ATOM	2554	CA	ILE	B	751	15.355	2.641	36.304	1.00	9.43	C
ATOM	2555	C	ILE	B	751	15.837	2.740	34.869	1.00	8.46	C
ATOM	2556	O	ILE	B	751	15.288	3.563	34.169	1.00	5.95	O
ATOM	2557	CB	ILE	B	751	16.165	3.345	37.407	1.00	3.46	C
ATOM	2558	CG1	ILE	B	751	15.174	3.285	38.624	1.00	2.83	C
ATOM	2559	CG2	ILE	B	751	16.496	4.749	36.947	1.00	2.42	C
ATOM	2560	CD1	ILE	B	751	16.066	3.021	39.864	1.00	4.21	C
ATOM	2561	N	GLN	B	752	16.784	2.046	34.310	1.00	10.70	N

FIG. 7 CONT'D

ATOM	2562	CA	GLN	B	752	17.200	2.304	32.933	1.00	13.10	C
ATOM	2563	C	GLN	B	752	16.109	2.359	31.879	1.00	13.51	C
ATOM	2564	O	GLN	B	752	16.075	3.250	31.083	1.00	13.45	O
ATOM	2565	CB	GLN	B	752	18.381	1.383	32.641	1.00	8.29	C
ATOM	2566	CG	GLN	B	752	19.487	1.736	33.603	1.00	7.41	C
ATOM	2567	CD	GLN	B	752	20.808	1.191	33.061	1.00	8.86	C
ATOM	2568	OE1	GLN	B	752	21.814	1.897	33.241	1.00	5.08	O
ATOM	2569	NE2	GLN	B	752	20.623	0.013	32.476	1.00	9.69	N
ATOM	2570	N	TYR	B	753	15.158	1.473	31.872	1.00	13.07	N
ATOM	2571	CA	TYR	B	753	13.904	1.323	31.273	1.00	10.75	C
ATOM	2572	C	TYR	B	753	12.963	2.404	31.706	1.00	10.33	C
ATOM	2573	O	TYR	B	753	12.151	2.670	30.852	1.00	9.92	O
ATOM	2574	CB	TYR	B	753	13.173	-0.039	31.322	1.00	2.02	C
ATOM	2575	CG	TYR	B	753	13.882	-1.273	30.779	1.00	6.31	C
ATOM	2576	CD1	TYR	B	753	15.195	-1.364	30.343	1.00	2.53	C
ATOM	2577	CD2	TYR	B	753	13.251	-2.535	30.839	1.00	9.38	C
ATOM	2578	CE1	TYR	B	753	15.762	-2.590	30.061	1.00	2.11	C
ATOM	2579	CE2	TYR	B	753	13.749	-3.775	30.463	1.00	6.47	C
ATOM	2580	CZ	TYR	B	753	15.023	-3.757	30.010	1.00	6.30	C
ATOM	2581	OH	TYR	B	753	15.726	-4.886	29.578	1.00	5.08	O
ATOM	2582	N	SER	B	754	12.781	3.069	32.788	1.00	13.02	N
ATOM	2583	CA	SER	B	754	11.654	4.024	32.882	1.00	13.02	C
ATOM	2584	C	SER	B	754	12.063	5.463	32.859	1.00	11.83	C
ATOM	2585	O	SER	B	754	11.083	6.182	33.011	1.00	7.98	O
ATOM	2586	CB	SER	B	754	10.716	3.777	34.049	1.00	13.17	C
ATOM	2587	OG	SER	B	754	11.300	3.843	35.348	1.00	12.33	O
ATOM	2588	N	TRP	B	755	13.308	5.816	32.624	1.00	14.36	N
ATOM	2589	CA	TRP	B	755	13.621	7.227	32.780	1.00	21.85	C
ATOM	2590	C	TRP	B	755	12.742	8.080	31.864	1.00	23.18	C
ATOM	2591	O	TRP	B	755	11.919	8.822	32.426	1.00	22.62	O
ATOM	2592	CB	TRP	B	755	15.062	7.618	32.698	1.00	23.68	C
ATOM	2593	CG	TRP	B	755	15.683	7.210	31.435	1.00	28.44	C
ATOM	2594	CD1	TRP	B	755	16.032	5.959	31.061	1.00	32.06	C
ATOM	2595	CD2	TRP	B	755	16.031	8.057	30.342	1.00	31.42	C
ATOM	2596	NE1	TRP	B	755	16.547	5.916	29.766	1.00	34.90	N
ATOM	2597	CE2	TRP	B	755	16.566	7.246	29.322	1.00	33.80	C
ATOM	2598	CE3	TRP	B	755	15.937	9.423	30.100	1.00	31.72	C
ATOM	2599	CZ2	TRP	B	755	16.996	7.773	28.090	1.00	32.70	C
ATOM	2600	CZ3	TRP	B	755	16.363	9.893	28.892	1.00	31.70	C
ATOM	2601	CH2	TRP	B	755	16.894	9.081	27.889	1.00	30.36	C
ATOM	2602	N	MET	B	756	12.787	7.937	30.532	1.00	21.30	N
ATOM	2603	CA	MET	B	756	11.991	8.753	29.658	1.00	17.61	C
ATOM	2604	C	MET	B	756	10.598	8.935	30.241	1.00	15.41	C
ATOM	2605	O	MET	B	756	10.131	10.053	30.334	1.00	13.48	O
ATOM	2606	CB	MET	B	756	11.875	8.376	28.149	1.00	15.02	C
ATOM	2607	CG	MET	B	756	11.483	9.405	27.131	1.00	9.26	C
ATOM	2608	SD	MET	B	756	12.833	10.674	26.898	1.00	8.78	S
ATOM	2609	CE	MET	B	756	14.042	9.512	26.120	1.00	3.85	C
ATOM	2610	N	SER	B	757	9.862	7.856	30.492	1.00	13.95	N
ATOM	2611	CA	SER	B	757	8.425	7.979	30.778	1.00	12.20	C
ATOM	2612	C	SER	B	757	8.280	8.756	32.101	1.00	14.86	C
ATOM	2613	O	SER	B	757	7.329	9.547	32.272	1.00	13.34	O
ATOM	2614	CB	SER	B	757	7.862	6.629	30.891	1.00	2.34	C
ATOM	2615	OG	SER	B	757	7.344	6.159	32.211	1.00	9.31	O
ATOM	2616	N	LEU	B	758	9.152	8.443	33.089	1.00	13.69	N
ATOM	2617	CA	LEU	B	758	9.196	9.213	34.281	1.00	13.54	C
ATOM	2618	C	LEU	B	758	9.350	10.705	34.021	1.00	18.14	C
ATOM	2619	O	LEU	B	758	8.637	11.585	34.529	1.00	23.09	O
ATOM	2620	CB	LEU	B	758	10.385	8.655	35.139	1.00	9.26	C
ATOM	2621	CG	LEU	B	758	10.080	7.352	35.874	1.00	2.69	C
ATOM	2622	CD1	LEU	B	758	11.298	6.778	36.536	1.00	2.36	C
ATOM	2623	CD2	LEU	B	758	8.796	7.472	36.635	1.00	2.02	C
ATOM	2624	N	MET	B	759	10.342	11.225	33.336	1.00	19.45	N
ATOM	2625	CA	MET	B	759	10.606	12.576	32.920	1.00	19.45	C

FIG. 7 CONT'D

ATOM	2626	C	MET	B	759	9.487	13.267	32.161	1.00	20.34	C
ATOM	2627	O	MET	B	759	9.122	14.428	32.318	1.00	20.42	O
ATOM	2628	CB	MET	B	759	11.900	12.577	32.044	1.00	19.55	C
ATOM	2629	CG	MET	B	759	13.062	13.325	32.741	1.00	18.07	C
ATOM	2630	SD	MET	B	759	14.568	12.729	32.010	1.00	17.44	S
ATOM	2631	CE	MET	B	759	14.653	11.129	32.863	1.00	20.66	C
ATOM	2632	N	VAL	B	760	8.895	12.467	31.266	1.00	19.89	N
ATOM	2633	CA	VAL	B	760	7.727	12.937	30.576	1.00	19.54	C
ATOM	2634	C	VAL	B	760	6.505	13.053	31.450	1.00	20.87	C
ATOM	2635	O	VAL	B	760	5.888	14.147	31.607	1.00	20.84	O
ATOM	2636	CB	VAL	B	760	7.535	12.234	29.236	1.00	17.03	C
ATOM	2637	CG1	VAL	B	760	6.359	11.353	29.332	1.00	15.19	C
ATOM	2638	CG2	VAL	B	760	7.262	13.391	28.240	1.00	17.09	C
ATOM	2639	N	PHE	B	761	6.105	12.028	32.153	1.00	21.99	N
ATOM	2640	CA	PHE	B	761	5.054	12.135	33.148	1.00	21.91	C
ATOM	2641	C	PHE	B	761	5.010	13.275	34.136	1.00	22.60	C
ATOM	2642	O	PHE	B	761	3.939	13.690	34.568	1.00	21.89	O
ATOM	2643	CB	PHE	B	761	5.071	10.832	33.974	1.00	15.40	C
ATOM	2644	CG	PHE	B	761	3.650	10.622	34.469	1.00	12.40	C
ATOM	2645	CD1	PHE	B	761	2.559	10.699	33.565	1.00	2.42	C
ATOM	2646	CD2	PHE	B	761	3.434	10.473	35.833	1.00	9.72	C
ATOM	2647	CE1	PHE	B	761	1.348	10.423	34.148	1.00	6.31	C
ATOM	2648	CE2	PHE	B	761	2.175	10.302	36.375	1.00	6.59	C
ATOM	2649	CZ	PHE	B	761	1.148	10.246	35.520	1.00	6.18	C
ATOM	2650	N	GLY	B	762	6.167	13.777	34.568	1.00	23.27	N
ATOM	2651	CA	GLY	B	762	6.326	14.817	35.550	1.00	20.64	C
ATOM	2652	C	GLY	B	762	6.469	16.168	34.937	1.00	20.81	C
ATOM	2653	O	GLY	B	762	5.987	17.175	35.438	1.00	21.06	O
ATOM	2654	N	LEU	B	763	7.161	16.292	33.805	1.00	22.59	N
ATOM	2655	CA	LEU	B	763	6.844	17.434	32.947	1.00	20.23	C
ATOM	2656	C	LEU	B	763	5.312	17.605	32.807	1.00	20.66	C
ATOM	2657	O	LEU	B	763	4.747	18.617	33.218	1.00	17.57	O
ATOM	2658	CB	LEU	B	763	7.543	17.285	31.606	1.00	17.31	C
ATOM	2659	CG	LEU	B	763	6.857	18.169	30.483	1.00	13.88	C
ATOM	2660	CD1	LEU	B	763	6.790	19.671	30.816	1.00	12.20	C
ATOM	2661	CD2	LEU	B	763	7.564	17.923	29.199	1.00	9.12	C
ATOM	2662	N	GLY	B	764	4.550	16.605	32.296	1.00	20.53	N
ATOM	2663	CA	GLY	B	764	3.093	16.655	32.420	1.00	21.67	C
ATOM	2664	C	GLY	B	764	2.669	17.413	33.695	1.00	23.47	C
ATOM	2665	O	GLY	B	764	1.821	18.312	33.650	1.00	22.47	O
ATOM	2666	N	TRP	B	765	3.130	16.920	34.885	1.00	21.96	N
ATOM	2667	CA	TRP	B	765	2.391	17.129	36.096	1.00	18.83	C
ATOM	2668	C	TRP	B	765	2.563	18.609	36.371	1.00	20.15	C
ATOM	2669	O	TRP	B	765	1.657	19.303	36.631	1.00	20.30	O
ATOM	2670	CB	TRP	B	765	2.933	16.321	37.278	1.00	15.03	C
ATOM	2671	CG	TRP	B	765	2.361	16.756	38.612	1.00	8.19	C
ATOM	2672	CD1	TRP	B	765	3.025	17.379	39.598	1.00	7.66	C
ATOM	2673	CD2	TRP	B	765	1.024	16.597	39.075	1.00	7.48	C
ATOM	2674	NE1	TRP	B	765	2.205	17.637	40.661	1.00	6.70	N
ATOM	2675	CE2	TRP	B	765	0.948	17.146	40.320	1.00	7.27	C
ATOM	2676	CE3	TRP	B	765	-0.124	15.975	38.575	1.00	7.50	C
ATOM	2677	CZ2	TRP	B	765	-0.219	17.105	41.071	1.00	6.67	C
ATOM	2678	CZ3	TRP	B	765	-1.312	16.049	39.294	1.00	2.50	C
ATOM	2679	CH2	TRP	B	765	-1.341	16.529	40.562	1.00	5.49	C
ATOM	2680	N	ARG	B	766	3.825	18.984	36.352	1.00	22.34	N
ATOM	2681	CA	ARG	B	766	4.381	20.267	36.582	1.00	22.53	C
ATOM	2682	C	ARG	B	766	3.745	21.253	35.624	1.00	23.52	C
ATOM	2683	O	ARG	B	766	3.811	22.440	35.885	1.00	26.07	O
ATOM	2684	CB	ARG	B	766	5.885	20.346	36.193	1.00	17.76	C
ATOM	2685	CG	ARG	B	766	6.766	20.640	37.370	1.00	14.97	C
ATOM	2686	CD	ARG	B	766	8.235	20.775	37.123	1.00	14.11	C
ATOM	2687	NE	ARG	B	766	9.003	20.094	36.123	1.00	14.54	N
ATOM	2688	CZ	ARG	B	766	9.128	18.844	35.664	1.00	13.59	C
ATOM	2689	NH1	ARG	B	766	8.362	17.982	36.279	1.00	11.42	N

FIG. 7 CONT'D

ATOM	2690	NH2	ARG	B	766	9.909	18.372	34.707	1.00	13.13	N
ATOM	2691	N	SER	B	767	3.403	20.920	34.426	1.00	23.57	N
ATOM	2692	CA	SER	B	767	2.975	21.956	33.506	1.00	24.17	C
ATOM	2693	C	SER	B	767	1.530	22.306	33.822	1.00	29.29	C
ATOM	2694	O	SER	B	767	1.077	23.477	33.894	1.00	28.86	O
ATOM	2695	CB	SER	B	767	3.339	21.596	32.083	1.00	17.40	C
ATOM	2696	OG	SER	B	767	4.623	22.179	32.028	1.00	7.81	O
ATOM	2697	N	TYR	B	768	0.796	21.225	34.075	1.00	31.05	N
ATOM	2698	CA	TYR	B	768	-0.541	21.303	34.585	1.00	31.41	C
ATOM	2699	C	TYR	B	768	-0.613	21.831	35.989	1.00	31.48	C
ATOM	2700	O	TYR	B	768	-1.647	22.477	36.125	1.00	33.09	O
ATOM	2701	CB	TYR	B	768	-1.191	19.977	34.447	1.00	32.03	C
ATOM	2702	CG	TYR	B	768	-2.328	19.637	35.381	1.00	34.81	C
ATOM	2703	CD1	TYR	B	768	-3.607	20.074	35.047	1.00	34.01	C
ATOM	2704	CD2	TYR	B	768	-2.128	18.879	36.565	1.00	33.99	C
ATOM	2705	CE1	TYR	B	768	-4.702	19.772	35.826	1.00	34.10	C
ATOM	2706	CE2	TYR	B	768	-3.241	18.594	37.332	1.00	33.94	C
ATOM	2707	CZ	TYR	B	768	-4.508	19.033	36.978	1.00	33.60	C
ATOM	2708	OH	TYR	B	768	-5.605	18.725	37.744	1.00	32.52	O
ATOM	2709	N	LYS	B	769	0.180	21.588	36.979	1.00	32.32	N
ATOM	2710	CA	LYS	B	769	0.190	22.347	38.211	1.00	36.21	C
ATOM	2711	C	LYS	B	769	0.504	23.868	38.198	1.00	37.30	C
ATOM	2712	O	LYS	B	769	-0.269	24.527	38.881	1.00	38.38	O
ATOM	2713	CB	LYS	B	769	1.216	21.886	39.313	1.00	35.58	C
ATOM	2714	CG	LYS	B	769	0.697	20.736	40.138	1.00	33.46	C
ATOM	2715	CD	LYS	B	769	0.263	20.877	41.551	1.00	32.31	C
ATOM	2716	CE	LYS	B	769	0.958	21.714	42.613	1.00	30.90	C
ATOM	2717	NZ	LYS	B	769	0.922	21.002	43.968	1.00	26.65	N
ATOM	2718	N	HIS	B	770	1.605	24.311	37.640	1.00	35.47	N
ATOM	2719	CA	HIS	B	770	2.123	25.610	37.560	1.00	34.20	C
ATOM	2720	C	HIS	B	770	1.744	26.564	36.448	1.00	34.17	C
ATOM	2721	O	HIS	B	770	2.082	27.774	36.577	1.00	34.57	O
ATOM	2722	CB	HIS	B	770	3.657	25.376	37.326	1.00	34.51	C
ATOM	2723	CG	HIS	B	770	4.393	24.826	38.518	1.00	36.08	C
ATOM	2724	ND1	HIS	B	770	4.691	25.534	39.703	1.00	33.16	N
ATOM	2725	CD2	HIS	B	770	4.880	23.561	38.689	1.00	34.81	C
ATOM	2726	CE1	HIS	B	770	5.327	24.736	40.479	1.00	31.67	C
ATOM	2727	NE2	HIS	B	770	5.471	23.542	39.917	1.00	33.57	N
ATOM	2728	N	VAL	B	771	1.300	26.200	35.242	1.00	31.81	N
ATOM	2729	CA	VAL	B	771	1.157	27.185	34.164	1.00	28.56	C
ATOM	2730	C	VAL	B	771	-0.020	26.726	33.330	1.00	30.77	C
ATOM	2731	O	VAL	B	771	-0.051	26.893	32.131	1.00	31.49	O
ATOM	2732	CB	VAL	B	771	2.414	27.402	33.319	1.00	26.19	C
ATOM	2733	CG1	VAL	B	771	3.415	28.320	34.059	1.00	23.78	C
ATOM	2734	CG2	VAL	B	771	3.174	26.201	32.804	1.00	20.57	C
ATOM	2735	N	SER	B	772	-0.855	25.874	33.943	1.00	30.02	N
ATOM	2736	CA	SER	B	772	-2.230	25.601	33.574	1.00	28.66	C
ATOM	2737	C	SER	B	772	-2.378	24.539	32.506	1.00	32.41	C
ATOM	2738	O	SER	B	772	-3.443	24.114	31.976	1.00	34.16	O
ATOM	2739	CB	SER	B	772	-2.869	26.941	33.272	1.00	25.15	C
ATOM	2740	OG	SER	B	772	-3.611	27.549	34.309	1.00	20.06	O
ATOM	2741	N	GLY	B	773	-1.219	24.001	32.151	1.00	34.20	N
ATOM	2742	CA	GLY	B	773	-1.123	23.037	31.037	1.00	32.86	C
ATOM	2743	C	GLY	B	773	-0.693	23.868	29.827	1.00	30.98	C
ATOM	2744	O	GLY	B	773	-0.547	23.333	28.740	1.00	29.04	O
ATOM	2745	N	GLN	B	774	-0.509	25.166	29.993	1.00	30.75	N
ATOM	2746	CA	GLN	B	774	-0.469	26.009	28.823	1.00	30.96	C
ATOM	2747	C	GLN	B	774	0.906	26.406	28.357	1.00	30.00	C
ATOM	2748	O	GLN	B	774	0.943	27.245	27.464	1.00	31.44	O
ATOM	2749	CB	GLN	B	774	-1.296	27.274	28.939	1.00	29.63	C
ATOM	2750	CG	GLN	B	774	-2.794	27.213	28.873	1.00	27.48	C
ATOM	2751	CD	GLN	B	774	-3.326	25.898	28.275	1.00	26.05	C
ATOM	2752	OE1	GLN	B	774	-3.181	25.744	27.048	1.00	22.82	O
ATOM	2753	NE2	GLN	B	774	-3.863	25.217	29.285	1.00	23.09	N

FIG. 7 CONT'D

ATOM	2754	N	MET	B	775	1.959	25.870	28.937	1.00	28.08	N
ATOM	2755	CA	MET	B	775	3.379	26.121	28.598	1.00	24.20	C
ATOM	2756	C	MET	B	775	4.118	24.865	29.013	1.00	20.59	C
ATOM	2757	O	MET	B	775	3.414	24.265	29.758	1.00	18.88	O
ATOM	2758	CB	MET	B	775	3.802	27.389	29.323	1.00	23.71	C
ATOM	2759	CG	MET	B	775	3.565	28.821	29.002	1.00	18.66	C
ATOM	2760	SD	MET	B	775	4.551	29.933	30.119	1.00	20.14	S
ATOM	2761	CE	MET	B	775	3.138	30.218	31.178	1.00	20.44	C
ATOM	2762	N	LEU	B	776	5.205	24.291	28.590	1.00	18.31	N
ATOM	2763	CA	LEU	B	776	5.913	23.178	29.081	1.00	15.72	C
ATOM	2764	C	LEU	B	776	6.880	23.578	30.219	1.00	20.60	C
ATOM	2765	O	LEU	B	776	7.809	24.313	29.970	1.00	21.33	O
ATOM	2766	CB	LEU	B	776	6.835	22.377	28.144	1.00	3.10	C
ATOM	2767	CG	LEU	B	776	5.887	21.986	27.022	1.00	6.88	C
ATOM	2768	CD1	LEU	B	776	6.454	21.594	25.660	1.00	6.40	C
ATOM	2769	CD2	LEU	B	776	4.919	20.905	27.507	1.00	2.35	C
ATOM	2770	N	TYR	B	777	6.639	23.089	31.444	1.00	22.28	N
ATOM	2771	CA	TYR	B	777	7.311	23.608	32.600	1.00	23.33	C
ATOM	2772	C	TYR	B	777	8.424	22.582	32.858	1.00	25.45	C
ATOM	2773	O	TYR	B	777	8.287	21.824	33.825	1.00	26.39	O
ATOM	2774	CB	TYR	B	777	6.380	23.755	33.811	1.00	20.42	C
ATOM	2775	CG	TYR	B	777	7.034	24.497	34.970	1.00	17.88	C
ATOM	2776	CD1	TYR	B	777	7.844	23.855	35.863	1.00	17.45	C
ATOM	2777	CD2	TYR	B	777	6.919	25.860	35.190	1.00	16.08	C
ATOM	2778	CE1	TYR	B	777	8.500	24.474	36.899	1.00	17.55	C
ATOM	2779	CE2	TYR	B	777	7.568	26.483	36.191	1.00	15.00	C
ATOM	2780	CZ	TYR	B	777	8.378	25.845	37.094	1.00	16.83	C
ATOM	2781	OH	TYR	B	777	9.072	26.458	38.170	1.00	14.24	O
ATOM	2782	N	PHE	B	778	9.403	22.481	31.957	1.00	24.20	N
ATOM	2783	CA	PHE	B	778	10.570	21.666	32.210	1.00	22.82	C
ATOM	2784	C	PHE	B	778	11.256	21.915	33.548	1.00	23.79	C
ATOM	2785	O	PHE	B	778	11.542	20.954	34.278	1.00	24.63	O
ATOM	2786	CB	PHE	B	778	11.619	21.716	31.111	1.00	16.95	C
ATOM	2787	CG	PHE	B	778	11.122	21.025	29.874	1.00	12.19	C
ATOM	2788	CD1	PHE	B	778	11.104	19.648	29.811	1.00	8.04	C
ATOM	2789	CD2	PHE	B	778	10.676	21.906	28.834	1.00	10.42	C
ATOM	2790	CE1	PHE	B	778	10.657	19.113	28.615	1.00	9.49	C
ATOM	2791	CE2	PHE	B	778	10.218	21.280	27.668	1.00	10.61	C
ATOM	2792	CZ	PHE	B	778	10.197	19.897	27.523	1.00	8.96	C
ATOM	2793	N	ALA	B	779	11.633	23.127	33.867	1.00	23.58	N
ATOM	2794	CA	ALA	B	779	12.054	23.559	35.199	1.00	20.96	C
ATOM	2795	C	ALA	B	779	11.609	24.991	35.465	1.00	21.45	C
ATOM	2796	O	ALA	B	779	11.285	25.851	34.594	1.00	16.49	O
ATOM	2797	CB	ALA	B	779	13.531	23.231	35.177	1.00	17.74	C
ATOM	2798	N	PRO	B	780	11.728	25.362	36.776	1.00	24.20	N
ATOM	2799	CA	PRO	B	780	11.658	26.820	37.077	1.00	26.98	C
ATOM	2800	C	PRO	B	780	12.486	27.656	36.110	1.00	30.00	C
ATOM	2801	O	PRO	B	780	11.991	28.612	35.474	1.00	33.83	O
ATOM	2802	CB	PRO	B	780	12.004	27.001	38.507	1.00	22.20	C
ATOM	2803	CG	PRO	B	780	12.577	25.681	38.849	1.00	23.60	C
ATOM	2804	CD	PRO	B	780	12.943	24.959	37.595	1.00	22.31	C
ATOM	2805	N	ASP	B	781	13.753	27.379	35.897	1.00	30.71	N
ATOM	2806	CA	ASP	B	781	14.486	28.044	34.847	1.00	29.94	C
ATOM	2807	C	ASP	B	781	14.371	27.567	33.436	1.00	28.66	C
ATOM	2808	O	ASP	B	781	15.177	28.114	32.637	1.00	30.84	O
ATOM	2809	CB	ASP	B	781	15.952	28.030	35.248	1.00	29.29	C
ATOM	2810	CG	ASP	B	781	16.529	26.639	35.154	1.00	28.78	C
ATOM	2811	OD1	ASP	B	781	15.772	25.688	35.420	1.00	28.01	O
ATOM	2812	OD2	ASP	B	781	17.732	26.618	34.808	1.00	28.47	O
ATOM	2813	N	LEU	B	782	13.495	26.657	33.048	1.00	25.87	N
ATOM	2814	CA	LEU	B	782	13.390	26.365	31.574	1.00	25.10	C
ATOM	2815	C	LEU	B	782	11.908	26.295	31.255	1.00	24.59	C
ATOM	2816	O	LEU	B	782	11.494	25.158	31.500	1.00	23.38	O
ATOM	2817	CB	LEU	B	782	13.892	25.017	30.982	1.00	19.11	C

FIG. 7 CONT'D

ATOM	2818	CG	LEU	B	782	14.359	24.804	29.553	1.00	12.78	C
ATOM	2819	CD1	LEU	B	782	15.244	26.011	29.139	1.00	12.09	C
ATOM	2820	CD2	LEU	B	782	15.297	23.640	29.391	1.00	2.11	C
ATOM	2821	N	ILE	B	783	11.211	27.339	30.926	1.00	25.58	N
ATOM	2822	CA	ILE	B	783	9.800	27.107	30.632	1.00	26.90	C
ATOM	2823	C	ILE	B	783	9.527	27.220	29.156	1.00	28.98	C
ATOM	2824	O	ILE	B	783	9.878	28.246	28.576	1.00	31.43	O
ATOM	2825	CB	ILE	B	783	9.054	28.122	31.494	1.00	24.13	C
ATOM	2826	CG1	ILE	B	783	9.261	27.679	32.937	1.00	24.47	C
ATOM	2827	CG2	ILE	B	783	7.552	28.076	31.145	1.00	23.74	C
ATOM	2828	CD1	ILE	B	783	8.716	28.637	33.976	1.00	24.36	C
ATOM	2829	N	LEU	B	784	8.944	26.341	28.398	1.00	31.45	N
ATOM	2830	CA	LEU	B	784	8.701	26.610	26.991	1.00	34.72	C
ATOM	2831	C	LEU	B	784	7.258	27.022	26.696	1.00	37.53	C
ATOM	2832	O	LEU	B	784	6.416	26.135	26.636	1.00	38.84	O
ATOM	2833	CB	LEU	B	784	8.964	25.456	26.013	1.00	31.39	C
ATOM	2834	CG	LEU	B	784	10.372	24.958	25.784	1.00	28.84	C
ATOM	2835	CD1	LEU	B	784	10.624	24.815	24.290	1.00	30.01	C
ATOM	2836	CD2	LEU	B	784	11.501	25.704	26.402	1.00	27.46	C
ATOM	2837	N	ASN	B	785	7.024	28.229	26.235	1.00	42.32	N
ATOM	2838	CA	ASN	B	785	5.836	28.649	25.485	1.00	45.46	C
ATOM	2839	C	ASN	B	785	5.889	28.351	23.995	1.00	45.58	C
ATOM	2840	O	ASN	B	785	6.855	27.827	23.471	1.00	43.57	O
ATOM	2841	CB	ASN	B	785	5.521	30.133	25.819	1.00	44.95	C
ATOM	2842	CG	ASN	B	785	6.402	31.180	25.179	1.00	45.26	C
ATOM	2843	OD1	ASN	B	785	7.103	30.927	24.177	1.00	45.16	O
ATOM	2844	ND2	ASN	B	785	6.499	32.414	25.665	1.00	44.97	N
ATOM	2845	N	GLU	B	786	4.840	28.703	23.272	1.00	48.48	N
ATOM	2846	CA	GLU	B	786	4.642	28.311	21.894	1.00	50.98	C
ATOM	2847	C	GLU	B	786	5.564	28.958	20.897	1.00	52.47	C
ATOM	2848	O	GLU	B	786	6.028	28.423	19.916	1.00	54.11	O
ATOM	2849	CB	GLU	B	786	3.188	28.544	21.490	1.00	50.08	C
ATOM	2850	CG	GLU	B	786	2.891	27.385	20.556	1.00	51.99	C
ATOM	2851	CD	GLU	B	786	1.440	27.065	20.318	1.00	52.48	C
ATOM	2852	OE1	GLU	B	786	0.702	27.983	20.763	1.00	52.93	O
ATOM	2853	OE2	GLU	B	786	1.210	25.983	19.718	1.00	51.51	O
ATOM	2854	N	GLN	B	787	5.947	30.149	21.191	1.00	53.42	N
ATOM	2855	CA	GLN	B	787	6.991	30.918	20.554	1.00	53.75	C
ATOM	2856	C	GLN	B	787	8.291	30.173	20.535	1.00	55.11	C
ATOM	2857	O	GLN	B	787	8.607	29.483	19.579	1.00	56.62	O
ATOM	2858	CB	GLN	B	787	6.988	32.185	21.434	1.00	55.00	C
ATOM	2859	CG	GLN	B	787	7.191	33.420	20.617	1.00	55.51	C
ATOM	2860	CD	GLN	B	787	6.217	33.535	19.467	1.00	57.44	C
ATOM	2861	OE1	GLN	B	787	6.518	34.313	18.538	1.00	57.35	O
ATOM	2862	NE2	GLN	B	787	5.049	32.851	19.483	1.00	58.58	N
ATOM	2863	N	ARG	B	788	9.118	30.299	21.561	1.00	54.42	N
ATOM	2864	CA	ARG	B	788	10.179	29.395	21.878	1.00	52.33	C
ATOM	2865	C	ARG	B	788	10.193	27.977	21.310	1.00	50.11	C
ATOM	2866	O	ARG	B	788	11.187	27.458	20.805	1.00	50.10	O
ATOM	2867	CB	ARG	B	788	9.878	29.358	23.402	1.00	52.03	C
ATOM	2868	CG	ARG	B	788	11.271	29.330	23.979	1.00	54.01	C
ATOM	2869	CD	ARG	B	788	11.419	28.540	25.261	1.00	53.12	C
ATOM	2870	NE	ARG	B	788	12.838	28.681	25.582	1.00	53.12	N
ATOM	2871	CZ	ARG	B	788	13.389	28.920	26.752	1.00	52.12	C
ATOM	2872	NH1	ARG	B	788	12.642	29.040	27.824	1.00	51.80	N
ATOM	2873	NH2	ARG	B	788	14.703	29.023	26.810	1.00	51.92	N
ATOM	2874	N	MET	B	789	9.109	27.267	21.553	1.00	42.42	N
ATOM	2875	CA	MET	B	789	8.626	26.160	20.792	1.00	40.43	C
ATOM	2876	C	MET	B	789	8.821	26.461	19.335	1.00	43.39	C
ATOM	2877	O	MET	B	789	9.981	26.340	18.933	1.00	41.46	O
ATOM	2878	CB	MET	B	789	7.245	25.728	21.286	1.00	35.22	C
ATOM	2879	CG	MET	B	789	7.205	24.860	22.594	1.00	27.06	C
ATOM	2880	SD	MET	B	789	5.530	24.084	22.712	1.00	18.85	S
ATOM	2881	CE	MET	B	789	5.224	24.325	24.433	1.00	25.22	C

FIG. 7 CONT'D

ATOM	2882	N	LYS	B	790	7.901	27.019	18.554	1.00	49.59	N
ATOM	2883	CA	LYS	B	790	7.920	27.356	17.152	1.00	53.66	C
ATOM	2884	C	LYS	B	790	9.250	27.138	16.438	1.00	55.59	C
ATOM	2885	O	LYS	B	790	9.404	26.449	15.451	1.00	54.99	O
ATOM	2886	CB	LYS	B	790	7.524	28.803	16.823	1.00	58.38	C
ATOM	2887	CG	LYS	B	790	8.454	30.000	16.839	1.00	62.98	C
ATOM	2888	CD	LYS	B	790	8.102	31.467	16.812	1.00	64.35	C
ATOM	2889	CE	LYS	B	790	8.706	32.470	17.750	1.00	64.80	C
ATOM	2890	NZ	LYS	B	790	9.583	33.615	17.398	1.00	65.89	N
ATOM	2897	N	GLU	B	791	10.240	27.883	16.928	1.00	59.01	N
ATOM	2891	CA	GLU	B	791	11.512	28.180	16.325	1.00	60.26	C
ATOM	2898	C	GLU	B	791	12.562	27.372	17.075	1.00	59.57	C
ATOM	2899	O	GLU	B	791	13.515	28.084	17.362	1.00	59.58	O
ATOM	2892	CB	GLU	B	791	11.812	29.690	16.396	1.00	61.44	C
ATOM	2893	CG	GLU	B	791	11.331	30.541	15.230	1.00	64.18	C
ATOM	2894	CD	GLU	B	791	11.407	32.023	14.964	1.00	63.81	C
ATOM	2895	OE1	GLU	B	791	12.014	32.873	15.686	1.00	64.39	OE2 O
ATOM	2896	OE2	GLU	B	791	10.825	32.479	13.921	1.00	61.58	OE1 O
ATOM	2800	N	SER	B	792	12.356	26.093	17.336	1.00	58.96	N
ATOM	2901	CA	SER	B	792	13.161	25.386	18.318	1.00	60.47	C
ATOM	2904	C	SER	B	792	13.885	24.146	17.800	1.00	61.28	C
ATOM	2905	O	SER	B	792	14.807	23.637	18.423	1.00	60.51	O
ATOM	2902	CB	SER	B	792	12.329	24.856	19.496	1.00	60.59	C
ATOM	2903	OG	SER	B	792	11.217	24.071	19.068	1.00	60.51	O
ATOM	2906	N	SER	B	793	13.349	23.537	16.740	1.00	62.28	N
ATOM	2907	CA	SER	B	793	13.772	22.390	15.980	1.00	59.38	C
ATOM	2910	C	SER	B	793	13.055	21.094	16.395	1.00	59.29	C
ATOM	2911	O	SER	B	793	13.338	19.956	15.956	1.00	59.26	O
ATOM	2908	CB	SER	B	793	15.268	22.092	16.046	1.00	58.77	C
ATOM	2909	OG	SER	B	793	15.486	21.177	17.131	1.00	58.35	O
ATOM	2912	N	PHE	B	794	12.082	21.293	17.298	1.00	56.76	N
ATOM	2913	CA	PHE	B	794	11.438	20.101	17.848	1.00	53.98	C
ATOM	2914	C	PHE	B	794	10.083	20.449	18.381	1.00	52.47	C
ATOM	2915	O	PHE	B	794	9.331	19.776	19.089	1.00	52.94	O
ATOM	2916	CB	PHE	B	794	12.483	19.449	18.723	1.00	53.99	C
ATOM	2917	CG	PHE	B	794	12.813	20.036	20.049	1.00	52.79	C
ATOM	2918	CD1	PHE	B	794	11.952	19.835	21.112	1.00	51.28	CD2 C
ATOM	2919	CD2	PHE	B	794	13.994	20.776	20.193	1.00	52.69	CD1 C
ATOM	2920	CE1	PHE	B	794	12.314	20.392	22.323	1.00	53.40	CE2 C
ATOM	2921	CE2	PHE	B	794	14.334	21.333	21.405	1.00	51.61	CE1 C
ATOM	2922	CZ	PHE	B	794	13.494	21.124	22.484	1.00	52.92	C
ATOM	2923	N	TYR	B	795	9.511	21.498	17.791	1.00	51.98	N
ATOM	2924	CA	TYR	B	795	8.097	21.854	17.948	1.00	50.02	C
ATOM	2925	C	TYR	B	795	7.203	20.620	17.824	1.00	47.15	C
ATOM	2926	O	TYR	B	795	6.224	20.519	18.550	1.00	44.52	O
ATOM	2927	CB	TYR	B	795	7.687	22.940	16.942	1.00	50.67	C
ATOM	2928	CG	TYR	B	795	6.239	23.360	17.090	1.00	51.96	C
ATOM	2929	CD1	TYR	B	795	5.775	23.816	18.328	1.00	53.04	C
ATOM	2930	CD2	TYR	B	795	5.293	23.257	16.068	1.00	50.61	C
ATOM	2931	CE1	TYR	B	795	4.443	24.197	18.488	1.00	52.73	C
ATOM	2932	CE2	TYR	B	795	3.975	23.606	16.219	1.00	48.73	C
ATOM	2933	CZ	TYR	B	795	3.555	24.092	17.430	1.00	51.21	C
ATOM	2934	OH	TYR	B	795	2.271	24.507	17.724	1.00	52.07	O
ATOM	2935	N	SER	B	796	7.525	19.702	16.928	1.00	45.93	N
ATOM	2936	CA	SER	B	796	6.695	18.577	16.630	1.00	45.44	C
ATOM	2937	C	SER	B	796	6.773	17.526	17.727	1.00	46.09	C
ATOM	2938	O	SER	B	796	5.818	16.753	17.932	1.00	46.52	O
ATOM	2939	CB	SER	B	796	7.201	18.008	15.310	1.00	44.49	C
ATOM	2940	OG	SER	B	796	6.260	17.068	14.866	1.00	44.33	O
ATOM	2941	N	LEU	B	797	7.993	17.547	18.339	1.00	42.89	N
ATOM	2942	CA	LEU	B	797	8.173	16.772	19.556	1.00	39.09	C
ATOM	2943	C	LEU	B	797	7.456	17.493	20.695	1.00	37.45	C
ATOM	2944	O	LEU	B	797	6.516	16.975	21.314	1.00	38.11	O
ATOM	2945	CB	LEU	B	797	9.627	16.544	19.976	1.00	35.66	C

FIG. 7 CONT'D

ATOM	2946	CG	LEU	B	797	9.865	15.315	20.889	1.00	30.84	C
ATOM	2947	CD1	LEU	B	797	9.976	14.096	19.994	1.00	26.43	C
ATOM	2948	CD2	LEU	B	797	11.063	15.613	21.769	1.00	29.09	C
ATOM	2949	N	CYS	B	798	7.846	18.748	20.886	1.00	35.07	N
ATOM	2950	CA	CYS	B	798	7.108	19.530	21.882	1.00	35.16	C
ATOM	2951	C	CYS	B	798	5.586	19.441	21.868	1.00	36.90	C
ATOM	2952	O	CYS	B	798	5.028	19.348	22.981	1.00	37.84	O
ATOM	2953	CB	CYS	B	798	7.309	21.025	21.810	1.00	31.90	C
ATOM	2954	SG	CYS	B	798	9.037	21.418	22.134	1.00	31.65	S
ATOM	2955	N	LEU	B	799	4.924	19.473	20.719	1.00	37.61	N
ATOM	2956	CA	LEU	B	799	3.486	19.213	20.696	1.00	37.51	C
ATOM	2957	C	LEU	B	799	3.187	17.843	21.245	1.00	39.67	C
ATOM	2958	O	LEU	B	799	2.265	17.860	22.074	1.00	40.58	O
ATOM	2959	CB	LEU	B	799	2.901	19.616	19.365	1.00	35.01	C
ATOM	2960	CG	LEU	B	799	2.726	21.011	18.725	1.00	31.09	C
ATOM	2961	CD1	LEU	B	799	2.475	20.896	17.245	1.00	27.14	C
ATOM	2962	CD2	LEU	B	799	1.621	21.931	19.244	1.00	27.62	C
ATOM	2963	N	THR	B	800	3.925	16.766	20.980	1.00	39.89	N
ATOM	2964	CA	THR	B	800	3.643	15.458	21.575	1.00	38.73	C
ATOM	2965	C	THR	B	800	3.728	15.364	23.111	1.00	36.28	C
ATOM	2966	O	THR	B	800	2.922	14.777	23.854	1.00	33.56	O
ATOM	2967	CB	THR	B	800	4.667	14.468	20.960	1.00	39.15	C
ATOM	2968	OG1	THR	B	800	4.563	14.416	19.556	1.00	38.85	O
ATOM	2969	CG2	THR	B	800	4.547	13.071	21.570	1.00	40.19	C
ATOM	2970	N	MET	B	801	4.791	15.962	23.637	1.00	32.60	N
ATOM	2971	CA	MET	B	801	5.035	16.114	25.048	1.00	31.40	C
ATOM	2972	C	MET	B	801	3.903	16.785	25.733	1.00	34.26	C
ATOM	2973	O	MET	B	801	3.239	16.362	26.630	1.00	32.67	O
ATOM	2974	CB	MET	B	801	6.312	16.975	25.082	1.00	29.00	C
ATOM	2975	CG	MET	B	801	7.317	16.135	24.255	1.00	25.45	C
ATOM	2976	SD	MET	B	801	8.947	16.354	24.938	1.00	20.65	S
ATOM	2977	CE	MET	B	801	9.502	17.571	23.746	1.00	21.57	C
ATOM	2978	N	TRP	B	802	3.478	17.900	25.196	1.00	40.02	N
ATOM	2979	CA	TRP	B	802	2.283	18.697	25.499	1.00	41.26	C
ATOM	2980	C	TRP	B	802	0.982	17.907	25.611	1.00	43.30	C
ATOM	2981	O	TRP	B	802	0.031	18.321	26.287	1.00	42.08	O
ATOM	2982	CB	TRP	B	802	2.273	19.875	24.493	1.00	39.40	C
ATOM	2983	CG	TRP	B	802	1.781	21.226	24.939	1.00	38.13	C
ATOM	2984	CD1	TRP	B	802	1.565	21.551	26.251	1.00	38.05	C
ATOM	2985	CD2	TRP	B	802	1.464	22.426	24.219	1.00	36.15	C
ATOM	2986	NE1	TRP	B	802	1.118	22.824	26.395	1.00	35.96	N
ATOM	2987	CE2	TRP	B	802	1.059	23.396	25.158	1.00	36.26	C
ATOM	2988	CE3	TRP	B	802	1.492	22.804	22.875	1.00	34.87	C
ATOM	2989	CZ2	TRP	B	802	0.649	24.704	24.827	1.00	35.28	C
ATOM	2990	CZ3	TRP	B	802	1.082	24.096	22.569	1.00	35.07	C
ATOM	2991	CH2	TRP	B	802	0.660	25.045	23.503	1.00	33.91	C
ATOM	2992	N	GLN	B	803	0.847	16.707	25.073	1.00	44.21	N
ATOM	2993	CA	GLN	B	803	-0.358	15.911	25.205	1.00	43.44	C
ATOM	2994	C	GLN	B	803	-0.714	15.547	26.636	1.00	41.05	C
ATOM	2995	O	GLN	B	803	-1.840	15.537	27.156	1.00	38.76	O
ATOM	2996	CB	GLN	B	803	-0.015	14.728	24.322	1.00	45.80	C
ATOM	2997	CG	GLN	B	803	-0.047	15.085	22.850	1.00	49.15	C
ATOM	2998	CD	GLN	B	803	0.392	13.937	21.921	1.00	52.45	C
ATOM	2999	OE1	GLN	B	803	0.280	12.688	22.056	1.00	51.74	O
ATOM	3000	NE2	GLN	B	803	1.003	14.532	20.860	1.00	52.97	N
ATOM	3001	N	ILE	B	804	0.366	15.204	27.354	1.00	38.52	N
ATOM	3002	CA	ILE	B	804	0.273	14.816	28.750	1.00	33.62	C
ATOM	3003	C	ILE	B	804	-0.379	15.934	29.563	1.00	30.43	C
ATOM	3004	O	ILE	B	804	-1.484	15.710	30.084	1.00	28.55	O
ATOM	3005	CB	ILE	B	804	1.615	14.420	29.366	1.00	31.71	C
ATOM	3006	CG1	ILE	B	804	2.538	13.942	28.281	1.00	29.66	C
ATOM	3007	CG2	ILE	B	804	1.263	13.441	30.488	1.00	31.41	C
ATOM	3008	CD1	ILE	B	804	2.757	12.460	28.330	1.00	33.93	C
ATOM	3009	N	PRO	B	805	0.174	17.140	29.583	1.00	26.79	N

FIG. 7 CONT'D

ATOM	3010	CA	PRO	B	805	-0.353	18.189	30.391	1.00	28.45	C
ATOM	3011	C	PRO	B	805	-1.827	18.423	30.188	1.00	31.93	C
ATOM	3012	O	PRO	B	805	-2.601	18.759	31.080	1.00	33.17	O
ATOM	3013	CB	PRO	B	805	0.448	19.428	29.988	1.00	24.88	C
ATOM	3014	CG	PRO	B	805	1.677	18.950	29.294	1.00	22.11	C
ATOM	3015	CD	PRO	B	805	1.508	17.492	29.096	1.00	23.48	C
ATOM	3016	N	GLN	B	806	-2.277	18.194	28.949	1.00	35.43	N
ATOM	3017	CA	GLN	B	806	-3.611	18.471	28.470	1.00	36.67	C
ATOM	3018	C	GLN	B	806	-4.451	17.294	28.889	1.00	38.74	C
ATOM	3019	O	GLN	B	806	-5.605	17.548	29.283	1.00	42.08	O
ATOM	3020	CB	GLN	B	806	-3.514	18.910	27.020	1.00	35.94	C
ATOM	3021	CG	GLN	B	806	-2.440	19.912	26.649	1.00	35.60	C
ATOM	3022	CD	GLN	B	806	-2.709	21.367	26.921	1.00	35.15	C
ATOM	3023	OE1	GLN	B	806	-1.876	22.224	27.073	1.00	31.79	O
ATOM	3024	NE2	GLN	B	806	-3.968	21.761	27.005	1.00	36.71	N
ATOM	3025	N	GLU	B	807	-3.872	16.089	28.975	1.00	38.06	N
ATOM	3026	CA	GLU	B	807	-4.761	15.010	29.405	1.00	35.28	C
ATOM	3027	C	GLU	B	807	-5.080	15.025	30.885	1.00	32.67	C
ATOM	3028	O	GLU	B	807	-6.023	14.357	31.234	1.00	28.84	O
ATOM	3029	CB	GLU	B	807	-4.268	13.647	29.043	1.00	34.48	C
ATOM	3030	CG	GLU	B	807	-5.391	12.659	28.926	1.00	36.57	C
ATOM	3031	CD	GLU	B	807	-6.246	13.024	27.709	1.00	39.94	C
ATOM	3032	OE1	GLU	B	807	-5.843	13.970	26.951	1.00	38.15	O
ATOM	3033	OE2	GLU	B	807	-7.310	12.329	27.564	1.00	40.09	O
ATOM	3034	N	PHE	B	808	-4.330	15.803	31.618	1.00	33.16	N
ATOM	3035	CA	PHE	B	808	-4.263	15.957	33.062	1.00	34.32	C
ATOM	3036	C	PHE	B	808	-5.285	16.993	33.500	1.00	35.82	C
ATOM	3037	O	PHE	B	808	-6.021	16.958	34.464	1.00	35.52	O
ATOM	3038	CB	PHE	B	808	-2.901	16.526	33.545	1.00	29.79	C
ATOM	3039	CG	PHE	B	808	-1.837	15.488	33.706	1.00	26.09	C
ATOM	3040	CD1	PHE	B	808	-2.135	14.142	33.562	1.00	26.64	C
ATOM	3041	CD2	PHE	B	808	-0.553	15.803	34.022	1.00	24.02	C
ATOM	3042	CE1	PHE	B	808	-1.157	13.170	33.708	1.00	27.01	C
ATOM	3043	CE2	PHE	B	808	0.421	14.861	34.200	1.00	23.30	C
ATOM	3044	CZ	PHE	B	808	0.135	13.545	34.044	1.00	25.21	C
ATOM	3045	N	VAL	B	809	-5.246	17.997	32.605	1.00	37.37	N
ATOM	3046	CA	VAL	B	809	-6.133	19.161	32.690	1.00	36.19	C
ATOM	3047	C	VAL	B	809	-7.480	18.505	32.408	1.00	36.88	C
ATOM	3048	O	VAL	B	809	-8.432	18.633	33.119	1.00	36.56	O
ATOM	3049	CB	VAL	B	809	-5.927	20.339	31.751	1.00	33.10	C
ATOM	3050	CG1	VAL	B	809	-7.102	21.299	32.026	1.00	33.04	C
ATOM	3051	CG2	VAL	B	809	-4.681	21.219	31.803	1.00	29.95	C
ATOM	3052	N	LYS	B	810	-7.442	17.659	31.401	1.00	39.37	N
ATOM	3053	CA	LYS	B	810	-8.720	17.103	30.907	1.00	42.27	C
ATOM	3054	C	LYS	B	810	-9.247	16.269	32.049	1.00	44.17	C
ATOM	3055	O	LYS	B	810	-10.373	16.471	32.478	1.00	46.29	O
ATOM	3056	CB	LYS	B	810	-8.404	16.545	29.544	1.00	42.11	C
ATOM	3057	CG	LYS	B	810	-9.498	16.225	28.563	1.00	41.51	C
ATOM	3058	CD	LYS	B	810	-9.156	14.834	27.968	1.00	42.45	C
ATOM	3059	CE	LYS	B	810	-8.631	14.997	26.544	1.00	42.18	C
ATOM	3060	NZ	LYS	B	810	-8.378	13.807	25.727	1.00	39.33	N
ATOM	3061	N	LEU	B	811	-8.374	15.501	32.696	1.00	45.27	N
ATOM	3062	CA	LEU	B	811	-8.784	14.455	33.640	1.00	43.08	C
ATOM	3063	C	LEU	B	811	-8.987	14.960	35.045	1.00	41.97	C
ATOM	3064	O	LEU	B	811	-9.501	14.227	35.883	1.00	39.98	O
ATOM	3065	CB	LEU	B	811	-7.817	13.246	33.542	1.00	37.98	C
ATOM	3066	CG	LEU	B	811	-8.205	12.242	32.423	1.00	31.38	C
ATOM	3067	CD1	LEU	B	811	-7.176	11.189	32.174	1.00	29.61	C
ATOM	3068	CD2	LEU	B	811	-9.552	11.678	32.819	1.00	27.54	C
ATOM	3069	N	GLN	B	812	-8.600	16.214	35.302	1.00	42.45	N
ATOM	3070	CA	GLN	B	812	-8.483	16.646	36.708	1.00	44.30	C
ATOM	3071	C	GLN	B	812	-7.885	15.584	37.656	1.00	45.08	C
ATOM	3072	O	GLN	B	812	-8.471	15.182	38.655	1.00	46.31	O
ATOM	3073	CB	GLN	B	812	-9.917	16.864	37.163	1.00	45.54	C

FIG. 7 CONT'D

ATOM	3074	CG	GLN	B	812	-10.676	18.162	37.094	1.00	47.24	C
ATOM	3075	CD	GLN	B	812	-12.203	17.945	37.028	1.00	48.81	C
ATOM	3076	OE1	GLN	B	812	-13.063	18.741	36.495	1.00	48.12	O
ATOM	3077	NE2	GLN	B	812	-12.586	16.766	37.576	1.00	47.42	N
ATOM	3078	N	VAL	B	813	-6.767	14.923	37.408	1.00	42.10	N
ATOM	3079	CA	VAL	B	813	-5.721	14.305	38.104	1.00	35.75	C
ATOM	3080	C	VAL	B	813	-5.121	15.088	39.311	1.00	34.98	C
ATOM	3081	O	VAL	B	813	-4.606	16.253	39.462	1.00	29.86	O
ATOM	3082	CB	VAL	B	813	-4.486	14.061	37.209	1.00	34.98	C
ATOM	3083	CG1	VAL	B	813	-3.722	12.855	37.715	1.00	34.59	C
ATOM	3084	CG2	VAL	B	813	-4.883	13.873	35.751	1.00	34.45	C
ATOM	3085	N	SER	B	814	-5.320	14.185	40.345	1.00	32.92	N
ATOM	3086	CA	SER	B	814	-5.041	14.660	41.728	1.00	31.86	C
ATOM	3087	C	SER	B	814	-3.595	14.370	42.058	1.00	33.45	C
ATOM	3088	O	SER	B	814	-3.066	13.341	41.538	1.00	33.13	O
ATOM	3089	CB	SER	B	814	-6.111	13.900	42.472	1.00	30.15	C
ATOM	3090	OG	SER	B	814	-5.858	12.612	43.006	1.00	30.40	O
ATOM	3091	N	GLN	B	815	-2.937	15.119	42.944	1.00	34.48	N
ATOM	3092	CA	GLN	B	815	-1.747	14.635	43.651	1.00	38.27	C
ATOM	3093	C	GLN	B	815	-1.647	13.131	44.016	1.00	39.64	C
ATOM	3094	O	GLN	B	815	-0.580	12.475	43.903	1.00	40.57	O
ATOM	3095	CB	GLN	B	815	-1.517	15.316	45.011	1.00	37.53	C
ATOM	3096	CG	GLN	B	815	-0.264	14.757	45.693	1.00	39.60	C
ATOM	3097	CD	GLN	B	815	0.994	15.527	45.420	1.00	41.10	C
ATOM	3098	OE1	GLN	B	815	1.908	15.397	44.623	1.00	41.70	O
ATOM	3099	NE2	GLN	B	815	1.004	16.513	46.332	1.00	41.86	N
ATOM	3100	N	GLU	B	816	-2.739	12.569	44.551	1.00	38.55	N
ATOM	3101	CA	GLU	B	816	-2.696	11.259	45.145	1.00	36.65	C
ATOM	3102	C	GLU	B	816	-2.512	10.280	44.028	1.00	35.88	C
ATOM	3103	O	GLU	B	816	-1.626	9.429	44.124	1.00	36.30	O
ATOM	3104	CB	GLU	B	816	-3.939	11.008	45.972	1.00	34.60	C
ATOM	3105	CG	GLU	B	816	-3.936	11.986	47.152	1.00	31.57	C
ATOM	3106	CD	GLU	B	816	-4.517	13.333	46.923	1.00	30.95	C
ATOM	3107	OE1	GLU	B	816	-5.401	13.593	46.083	1.00	29.33	O
ATOM	3108	OE2	GLU	B	816	-4.152	14.242	47.682	1.00	32.85	O
ATOM	3109	N	GLU	B	817	-3.275	10.595	42.963	1.00	34.38	N
ATOM	3110	CA	GLU	B	817	-3.282	9.592	41.848	1.00	32.53	C
ATOM	3111	C	GLU	B	817	-2.017	9.784	41.035	1.00	32.15	C
ATOM	3112	O	GLU	B	817	-1.409	8.735	40.786	1.00	33.94	O
ATOM	3113	CB	GLU	B	817	-4.537	9.638	41.069	1.00	30.26	C
ATOM	3114	CG	GLU	B	817	-5.783	9.838	41.926	1.00	30.04	C
ATOM	3115	CD	GLU	B	817	-7.004	10.134	41.106	1.00	30.78	C
ATOM	3116	OE1	GLU	B	817	-6.959	10.940	40.185	1.00	29.71	O
ATOM	3117	OE2	GLU	B	817	-8.043	9.460	41.338	1.00	33.33	O
ATOM	3118	N	PHE	B	818	-1.528	11.040	40.887	1.00	28.40	N
ATOM	3119	CA	PHE	B	818	-0.221	11.277	40.321	1.00	22.83	C
ATOM	3120	C	PHE	B	818	0.868	10.504	41.002	1.00	20.86	C
ATOM	3121	O	PHE	B	818	1.542	9.789	40.294	1.00	20.70	O
ATOM	3122	CB	PHE	B	818	0.303	12.686	40.306	1.00	22.32	C
ATOM	3123	CG	PHE	B	818	1.679	12.939	39.760	1.00	23.86	C
ATOM	3124	CD1	PHE	B	818	1.982	12.911	38.409	1.00	25.28	C
ATOM	3125	CD2	PHE	B	818	2.751	13.208	40.574	1.00	23.28	C
ATOM	3126	CE1	PHE	B	818	3.232	13.159	37.887	1.00	23.69	C
ATOM	3127	CE2	PHE	B	818	4.002	13.547	40.124	1.00	22.04	C
ATOM	3128	CZ	PHE	B	818	4.231	13.534	38.778	1.00	23.67	C
ATOM	3129	N	LEU	B	819	1.009	10.719	42.310	1.00	16.75	N
ATOM	3130	CA	LEU	B	819	1.950	9.892	43.094	1.00	11.74	C
ATOM	3131	C	LEU	B	819	1.814	8.401	42.871	1.00	9.53	C
ATOM	3132	O	LEU	B	819	2.871	7.862	42.482	1.00	8.43	O
ATOM	3133	CB	LEU	B	819	1.932	10.385	44.513	1.00	8.92	C
ATOM	3134	CG	LEU	B	819	2.626	11.693	44.811	1.00	11.05	C
ATOM	3135	CD1	LEU	B	819	2.445	11.973	46.343	1.00	9.50	C
ATOM	3136	CD2	LEU	B	819	4.112	12.000	44.573	1.00	7.09	C
ATOM	3137	N	CYS	B	820	0.876	7.560	43.197	1.00	2.96	N

FIG. 7 CONT'D

ATOM	3138	CA	CYS	B	820	0.621	6.263	42.675	1.00	11.24	C
ATOM	3139	C	CYS	B	820	0.875	5.951	41.219	1.00	13.39	C
ATOM	3140	O	CYS	B	820	1.351	4.827	41.046	1.00	10.38	O
ATOM	3141	CB	CYS	B	820	-0.883	6.153	42.949	1.00	12.24	C
ATOM	3142	SG	CYS	B	820	-1.218	5.710	44.633	1.00	13.27	S
ATOM	3143	N	MET	B	821	0.620	6.896	40.236	1.00	16.31	N
ATOM	3144	CA	MET	B	821	0.635	6.305	38.871	1.00	15.25	C
ATOM	3145	C	MET	B	821	2.076	6.470	38.378	1.00	16.58	C
ATOM	3146	O	MET	B	821	2.609	5.726	37.555	1.00	16.62	O
ATOM	3147	CB	MET	B	821	-0.351	6.735	37.865	1.00	11.97	C
ATOM	3148	CG	MET	B	821	-1.793	7.068	38.161	1.00	10.89	C
ATOM	3149	SD	MET	B	821	-2.423	8.551	37.286	1.00	4.73	S
ATOM	3150	CE	MET	B	821	-2.862	7.660	35.736	1.00	6.16	C
ATOM	3151	N	LYS	B	822	2.693	7.447	39.082	1.00	16.93	N
ATOM	3152	CA	LYS	B	822	4.148	7.592	38.830	1.00	16.93	C
ATOM	3153	C	LYS	B	822	4.830	6.293	39.220	1.00	19.84	C
ATOM	3154	O	LYS	B	822	5.459	5.625	38.379	1.00	21.71	O
ATOM	3155	CB	LYS	B	822	4.601	8.942	39.362	1.00	10.49	C
ATOM	3156	CG	LYS	B	822	6.115	9.102	39.352	1.00	9.58	C
ATOM	3157	CD	LYS	B	822	6.618	10.514	39.275	1.00	6.81	C
ATOM	3158	CE	LYS	B	822	6.746	11.346	40.482	1.00	7.14	C
ATOM	3159	NZ	LYS	B	822	7.411	10.632	41.637	1.00	8.39	N
ATOM	3160	N	VAL	B	823	4.588	5.737	40.408	1.00	18.04	N
ATOM	3161	CA	VAL	B	823	5.270	4.536	40.867	1.00	13.65	C
ATOM	3162	C	VAL	B	823	4.954	3.443	39.842	1.00	13.96	C
ATOM	3163	O	VAL	B	823	5.925	2.778	39.462	1.00	14.64	O
ATOM	3164	CB	VAL	B	823	4.952	4.009	42.264	1.00	11.46	C
ATOM	3165	CG1	VAL	B	823	5.521	2.610	42.602	1.00	10.53	C
ATOM	3166	CG2	VAL	B	823	5.455	4.873	43.328	1.00	2.02	C
ATOM	3167	N	LEU	B	824	3.657	3.375	39.514	1.00	13.86	N
ATOM	3168	CA	LEU	B	824	3.285	2.488	38.408	1.00	14.66	C
ATOM	3169	C	LEU	B	824	4.079	2.619	37.140	1.00	17.58	C
ATOM	3170	O	LEU	B	824	4.447	1.519	36.720	1.00	19.63	O
ATOM	3171	CB	LEU	B	824	1.784	2.416	38.223	1.00	10.42	C
ATOM	3172	CG	LEU	B	824	1.118	1.451	39.285	1.00	5.99	C
ATOM	3173	CD1	LEU	B	824	-0.384	1.590	39.021	1.00	7.63	C
ATOM	3174	CD2	LEU	B	824	1.841	0.089	39.327	1.00	2.02	C
ATOM	3175	N	LEU	B	825	4.492	3.735	36.570	1.00	19.30	N
ATOM	3176	CA	LEU	B	825	5.519	3.864	35.552	1.00	17.91	C
ATOM	3177	C	LEU	B	825	6.942	3.360	35.855	1.00	17.03	C
ATOM	3178	O	LEU	B	825	7.721	2.996	34.974	1.00	17.24	O
ATOM	3179	CB	LEU	B	825	5.681	5.366	35.067	1.00	14.99	C
ATOM	3180	CG	LEU	B	825	4.711	6.020	34.119	1.00	10.79	C
ATOM	3181	CD1	LEU	B	825	5.114	7.318	33.526	1.00	3.07	C
ATOM	3182	CD2	LEU	B	825	4.197	4.964	33.150	1.00	9.03	C
ATOM	3183	N	LEU	B	826	7.398	3.498	37.110	1.00	15.12	N
ATOM	3184	CA	LEU	B	826	8.641	2.895	37.506	1.00	12.15	C
ATOM	3185	C	LEU	B	826	8.535	1.371	37.469	1.00	14.04	C
ATOM	3186	O	LEU	B	826	9.653	0.961	37.165	1.00	15.02	O
ATOM	3187	CB	LEU	B	826	9.212	3.341	38.838	1.00	7.24	C
ATOM	3188	CG	LEU	B	826	10.564	2.732	39.272	1.00	2.82	C
ATOM	3189	CD1	LEU	B	826	11.872	3.427	38.876	1.00	3.88	C
ATOM	3190	CD2	LEU	B	826	10.644	2.465	40.791	1.00	6.06	C
ATOM	3191	N	LEU	B	827	7.405	0.737	37.754	1.00	10.59	N
ATOM	3192	CA	LEU	B	827	7.218	-0.665	37.454	1.00	11.06	C
ATOM	3193	C	LEU	B	827	6.416	-1.033	36.151	1.00	16.62	C
ATOM	3194	O	LEU	B	827	5.761	-2.143	35.995	1.00	16.34	O
ATOM	3195	CB	LEU	B	827	6.532	-1.229	38.726	1.00	3.07	C
ATOM	3196	CG	LEU	B	827	6.935	-0.739	40.128	1.00	6.61	C
ATOM	3197	CD1	LEU	B	827	6.136	-1.279	41.315	1.00	2.32	C
ATOM	3198	CD2	LEU	B	827	8.310	-1.306	40.547	1.00	3.29	C
ATOM	3199	N	ASN	B	828	6.369	-0.130	35.113	1.00	18.13	N
ATOM	3200	CA	ASN	B	828	5.665	-0.520	33.945	1.00	22.96	C
ATOM	3201	C	ASN	B	828	6.237	-1.501	32.906	1.00	24.44	C

FIG. 7 CONT'D

ATOM	3202	O	ASN	B	828	5.298	-1.853	32.190	1.00	23.13	O
ATOM	3203	CB	ASN	B	828	5.141	0.610	33.083	1.00	24.96	C
ATOM	3204	CG	ASN	B	828	3.603	0.522	33.086	1.00	25.57	C
ATOM	3205	OD1	ASN	B	828	2.947	1.494	32.567	1.00	25.87	O
ATOM	3206	ND2	ASN	B	828	3.196	-0.578	33.690	1.00	20.40	N
ATOM	3207	N	THR	B	829	7.453	-1.957	32.847	1.00	25.54	N
ATOM	3208	CA	THR	B	829	8.118	-2.511	31.716	1.00	28.74	C
ATOM	3209	C	THR	B	829	9.157	-3.511	32.188	1.00	30.21	C
ATOM	3210	O	THR	B	829	10.014	-2.979	32.863	1.00	32.23	O
ATOM	3211	CB	THR	B	829	8.888	-1.433	30.912	1.00	29.41	C
ATOM	3212	OG1	THR	B	829	8.053	-0.349	30.444	1.00	28.42	O
ATOM	3213	CG2	THR	B	829	9.723	-2.027	29.777	1.00	29.02	C
ATOM	3214	N	ILE	B	830	9.286	-4.785	32.025	1.00	31.79	N
ATOM	3215	CA	ILE	B	830	10.546	-5.439	32.282	1.00	34.07	C
ATOM	3216	C	ILE	B	830	11.112	-6.133	31.081	1.00	35.38	C
ATOM	3217	O	ILE	B	830	10.331	-6.199	30.127	1.00	36.12	O
ATOM	3218	CB	ILE	B	830	10.378	-6.365	33.483	1.00	33.65	C
ATOM	3219	CG1	ILE	B	830	8.998	-6.586	34.064	1.00	32.78	C
ATOM	3220	CG2	ILE	B	830	11.245	-5.615	34.470	1.00	37.00	C
ATOM	3221	CD1	ILE	B	830	8.606	-5.543	35.095	1.00	29.17	C
ATOM	3222	N	PRO	B	831	12.277	-6.753	31.173	1.00	36.34	N
ATOM	3223	CA	PRO	B	831	12.766	-7.627	30.114	1.00	38.14	C
ATOM	3224	C	PRO	B	831	11.814	-8.772	29.792	1.00	40.98	C
ATOM	3225	O	PRO	B	831	11.005	-9.182	30.626	1.00	41.34	O
ATOM	3226	CB	PRO	B	831	14.055	-8.213	30.657	1.00	36.29	C
ATOM	3227	CG	PRO	B	831	14.248	-7.541	31.951	1.00	33.36	C
ATOM	3228	CD	PRO	B	831	12.812	-7.381	32.417	1.00	33.39	C
ATOM	3229	N	LEU	B	832	11.934	-9.270	28.562	1.00	43.04	N
ATOM	3230	CA	LEU	B	832	11.271	-10.475	28.101	1.00	44.84	C
ATOM	3231	C	LEU	B	832	11.592	-11.742	28.903	1.00	46.84	C
ATOM	3232	O	LEU	B	832	10.778	-12.660	28.823	1.00	48.06	O
ATOM	3233	CB	LEU	B	832	11.602	-10.869	26.647	1.00	41.14	C
ATOM	3234	CG	LEU	B	832	11.962	-9.765	25.652	1.00	38.20	C
ATOM	3235	CD1	LEU	B	832	12.895	-10.378	24.624	1.00	35.51	C
ATOM	3236	CD2	LEU	B	832	10.784	-9.022	25.063	1.00	34.95	C
ATOM	3237	N	GLU	B	833	12.703	-11.840	29.606	1.00	47.85	N
ATOM	3238	CA	GLU	B	833	13.031	-12.949	30.465	1.00	47.55	C
ATOM	3239	C	GLU	B	833	12.432	-12.789	31.868	1.00	46.68	C
ATOM	3240	O	GLU	B	833	12.743	-13.656	32.714	1.00	48.93	O
ATOM	3241	CB	GLU	B	833	14.531	-13.182	30.808	1.00	46.86	C
ATOM	3242	CG	GLU	B	833	15.604	-12.784	29.843	1.00	46.75	C
ATOM	3243	CD	GLU	B	833	15.665	-11.309	29.425	1.00	44.50	C
ATOM	3244	OE1	GLU	B	833	16.231	-10.522	30.199	1.00	43.48	O
ATOM	3245	OE2	GLU	B	833	15.208	-10.959	28.335	1.00	40.60	O
ATOM	3246	N	GLY	B	834	11.734	-11.716	32.143	1.00	43.40	N
ATOM	3247	CA	GLY	B	834	11.403	-11.273	33.466	1.00	39.05	C
ATOM	3248	C	GLY	B	834	12.567	-10.752	34.276	1.00	39.30	C
ATOM	3249	O	GLY	B	834	13.741	-10.816	33.892	1.00	38.69	O
ATOM	3250	N	LEU	B	835	12.297	-10.281	35.503	1.00	39.60	N
ATOM	3251	CA	LEU	B	835	13.269	-9.860	36.517	1.00	37.78	C
ATOM	3252	C	LEU	B	835	13.960	-10.964	37.284	1.00	37.86	C
ATOM	3253	O	LEU	B	835	13.488	-12.117	37.295	1.00	37.96	O
ATOM	3254	CB	LEU	B	835	12.580	-8.884	37.517	1.00	31.77	C
ATOM	3255	CG	LEU	B	835	12.496	-7.497	36.860	1.00	29.81	C
ATOM	3256	CD1	LEU	B	835	11.574	-6.525	37.582	1.00	28.33	C
ATOM	3257	CD2	LEU	B	835	13.842	-6.860	36.533	1.00	24.96	C
ATOM	3258	N	ARG	B	836	15.070	-10.673	37.966	1.00	39.10	N
ATOM	3259	CA	ARG	B	836	15.532	-11.587	39.017	1.00	39.90	C
ATOM	3260	C	ARG	B	836	14.599	-11.685	40.199	1.00	36.98	C
ATOM	3261	O	ARG	B	836	14.314	-12.792	40.557	1.00	40.99	O
ATOM	3262	CB	ARG	B	836	16.929	-11.357	39.592	1.00	41.35	C
ATOM	3263	CG	ARG	B	836	17.954	-11.270	38.469	1.00	44.43	C
ATOM	3264	CD	ARG	B	836	19.363	-11.115	39.020	1.00	45.63	C
ATOM	3265	NE	ARG	B	836	19.670	-12.265	39.836	1.00	48.41	N

FIG. 7 CONT'D

ATOM	3266	CZ	ARG	B	836	20.840	-12.366	40.458	1.00	50.38	C
ATOM	3267	NH1	ARG	B	836	21.664	-11.341	40.264	1.00	49.57	N
ATOM	3268	NH2	ARG	B	836	21.122	-13.410	41.251	1.00	50.42	N
ATOM	3269	N	SER	B	837	14.043	-10.777	40.876	1.00	31.98	N
ATOM	3270	CA	SER	B	837	13.031	-10.751	41.854	1.00	28.30	C
ATOM	3271	C	SER	B	837	11.597	-10.660	41.389	1.00	28.17	C
ATOM	3272	O	SER	B	837	10.759	-10.066	42.044	1.00	24.71	O
ATOM	3273	CB	SER	B	837	13.213	-9.471	42.706	1.00	29.97	C
ATOM	3274	OG	SER	B	837	14.284	-9.548	43.707	1.00	31.22	O
ATOM	3275	N	GLN	B	838	11.234	-11.287	40.304	1.00	28.72	N
ATOM	3276	CA	GLN	B	838	9.899	-11.263	39.813	1.00	29.37	C
ATOM	3277	C	GLN	B	838	8.921	-11.289	40.936	1.00	30.82	C
ATOM	3278	O	GLN	B	838	8.129	-10.373	41.077	1.00	34.01	O
ATOM	3279	CB	GLN	B	838	9.903	-12.300	38.704	1.00	25.32	C
ATOM	3280	CG	GLN	B	838	8.646	-12.119	37.874	1.00	25.16	C
ATOM	3281	CD	GLN	B	838	8.518	-10.714	37.264	1.00	24.09	C
ATOM	3282	OE1	GLN	B	838	7.448	-10.231	36.820	1.00	17.91	O
ATOM	3283	NE2	GLN	B	838	9.712	-10.064	37.274	1.00	25.01	N
ATOM	3284	N	THR	B	839	8.875	-12.248	41.811	1.00	31.99	N
ATOM	3285	CA	THR	B	839	7.810	-12.397	42.800	1.00	32.56	C
ATOM	3286	C	THR	B	839	7.575	-11.097	43.532	1.00	33.14	C
ATOM	3287	O	THR	B	839	6.542	-10.406	43.469	1.00	31.86	O
ATOM	3288	CB	THR	B	839	8.208	-13.662	43.583	1.00	32.53	C
ATOM	3289	OG1	THR	B	839	7.276	-14.648	43.122	1.00	32.88	O
ATOM	3290	CG2	THR	B	839	8.167	-13.663	45.108	1.00	31.69	C
ATOM	3291	N	GLN	B	840	8.575	-10.649	44.309	1.00	33.13	N
ATOM	3292	CA	GLN	B	840	8.723	-9.290	44.772	1.00	33.36	C
ATOM	3293	C	GLN	B	840	8.102	-8.209	43.912	1.00	30.16	C
ATOM	3294	O	GLN	B	840	7.217	-7.438	44.246	1.00	27.04	O
ATOM	3295	CB	GLN	B	840	10.251	-9.047	44.752	1.00	36.32	C
ATOM	3296	CG	GLN	B	840	10.873	-9.660	46.000	1.00	40.48	C
ATOM	3297	CD	GLN	B	840	12.100	-10.545	45.725	1.00	42.53	C
ATOM	3298	OE1	GLN	B	840	11.922	-11.701	45.292	1.00	42.25	O
ATOM	3299	NE2	GLN	B	840	13.338	-10.072	45.955	1.00	41.16	N
ATOM	3300	N	PHE	B	841	8.601	-8.161	42.695	1.00	27.17	N
ATOM	3301	CA	PHE	B	841	8.159	-7.262	41.626	1.00	23.94	C
ATOM	3302	C	PHE	B	841	6.655	-7.277	41.534	1.00	25.21	C
ATOM	3303	O	PHE	B	841	6.047	-6.228	41.556	1.00	22.06	O
ATOM	3304	CB	PHE	B	841	8.914	-7.500	40.303	1.00	15.95	C
ATOM	3305	CG	PHE	B	841	8.272	-6.566	39.355	1.00	13.95	C
ATOM	3306	CD1	PHE	B	841	7.123	-6.946	38.683	1.00	11.21	CD2 C
ATOM	3307	CD2	PHE	B	841	8.736	-5.269	39.132	1.00	12.57	CD1 C
ATOM	3308	CE1	PHE	B	841	6.461	-6.056	37.865	1.00	7.26	CE2 C
ATOM	3309	CE2	PHE	B	841	8.038	-4.388	38.343	1.00	8.34	CE1 C
ATOM	3310	CZ	PHE	B	841	6.933	-4.784	37.702	1.00	7.68	C
ATOM	3311	N	GLU	B	842	6.122	-8.504	41.491	1.00	29.17	N
ATOM	3312	CA	GLU	B	842	4.675	-8.599	41.254	1.00	33.33	C
ATOM	3313	C	GLU	B	842	3.960	-8.127	42.529	1.00	34.18	C
ATOM	3314	O	GLU	B	842	3.060	-7.270	42.558	1.00	31.70	O
ATOM	3315	CB	GLU	B	842	4.138	-9.861	40.622	1.00	34.77	C
ATOM	3316	CG	GLU	B	842	4.292	-10.313	39.193	1.00	37.08	C
ATOM	3317	CD	GLU	B	842	3.666	-9.699	37.981	1.00	37.70	C
ATOM	3318	OE1	GLU	B	842	2.603	-9.048	38.097	1.00	39.04	O
ATOM	3319	OE2	GLU	B	842	4.132	-9.777	36.805	1.00	39.35	O
ATOM	3320	N	GLU	B	843	4.444	-8.626	43.654	1.00	35.60	N
ATOM	3321	CA	GLU	B	843	3.938	-8.178	44.946	1.00	35.37	C
ATOM	3322	C	GLU	B	843	3.769	-6.684	45.131	1.00	32.56	C
ATOM	3323	O	GLU	B	843	2.759	-6.336	45.699	1.00	30.81	O
ATOM	3324	CB	GLU	B	843	4.949	-8.625	46.005	1.00	35.44	C
ATOM	3325	CG	GLU	B	843	5.064	-10.095	46.199	1.00	37.88	C
ATOM	3326	CD	GLU	B	843	4.921	-10.531	47.657	1.00	40.38	C
ATOM	3327	OE1	GLU	B	843	4.925	-9.512	48.411	1.00	40.45	O
ATOM	3328	OE2	GLU	B	843	4.840	-11.754	48.042	1.00	39.40	O
ATOM	3329	N	MET	B	844	4.795	-5.905	44.787	1.00	29.25	N

FIG. 7 CONT'D

ATOM	3330	CA	MET	B	844	4.872	-4.467	44.823	1.00	22.84	C
ATOM	3331	C	MET	B	844	3.993	-3.720	43.839	1.00	22.23	C
ATOM	3332	O	MET	B	844	3.396	-2.835	44.442	1.00	16.27	O
ATOM	3333	CB	MET	B	844	6.229	-3.883	44.511	1.00	15.87	C
ATOM	3334	CG	MET	B	844	6.379	-2.395	44.521	1.00	11.26	C
ATOM	3335	SD	MET	B	844	8.121	-1.973	44.592	1.00	3.00	S
ATOM	3336	CE	MET	B	844	7.924	-0.091	44.594	1.00	2.02	C
ATOM	3337	N	ARG	B	845	4.083	-4.184	42.581	1.00	24.18	N
ATOM	3338	CA	ARG	B	845	3.173	-3.694	41.535	1.00	25.42	C
ATOM	3339	C	ARG	B	845	1.720	-3.840	41.981	1.00	23.80	C
ATOM	3340	O	ARG	B	845	0.976	-2.872	41.816	1.00	22.73	O
ATOM	3341	CB	ARG	B	845	3.349	-4.244	40.129	1.00	26.65	C
ATOM	3342	CG	ARG	B	845	4.072	-3.756	38.953	1.00	30.20	C
ATOM	3343	CD	ARG	B	845	3.538	-3.769	37.553	1.00	37.32	C
ATOM	3344	NE	ARG	B	845	2.656	-3.333	36.528	1.00	37.79	N
ATOM	3345	CZ	ARG	B	845	1.488	-3.655	35.979	1.00	41.57	C
ATOM	3346	NH1	ARG	B	845	0.685	-4.665	36.326	1.00	41.33	N
ATOM	3347	NH2	ARG	B	845	0.934	-2.962	34.925	1.00	44.78	N
ATOM	3348	N	SER	B	846	1.276	-4.935	42.560	1.00	24.34	N
ATOM	3349	CA	SER	B	846	-0.062	-5.184	42.994	1.00	23.29	C
ATOM	3350	C	SER	B	846	-0.536	-4.241	44.083	1.00	25.33	C
ATOM	3351	O	SER	B	846	-1.607	-3.618	43.939	1.00	25.24	O
ATOM	3352	CB	SER	B	846	-0.321	-6.624	43.411	1.00	23.23	C
ATOM	3353	OG	SER	B	846	-0.045	-7.650	42.450	1.00	23.51	O
ATOM	3354	N	SER	B	847	0.295	-4.076	45.132	1.00	25.45	N
ATOM	3355	CA	SER	B	847	0.070	-3.178	46.228	1.00	22.84	C
ATOM	3356	C	SER	B	847	0.119	-1.763	45.744	1.00	22.68	C
ATOM	3357	O	SER	B	847	-0.541	-0.941	46.373	1.00	26.37	O
ATOM	3358	CB	SER	B	847	1.147	-3.279	47.296	1.00	24.84	C
ATOM	3359	OG	SER	B	847	1.079	-2.440	48.484	1.00	21.90	O
ATOM	3360	N	TYR	B	848	0.929	-1.357	44.811	1.00	20.56	N
ATOM	3361	CA	TYR	B	848	0.568	-0.061	44.248	1.00	20.37	C
ATOM	3362	C	TYR	B	848	-0.599	-0.016	43.304	1.00	20.34	C
ATOM	3363	O	TYR	B	848	-1.316	1.009	43.214	1.00	18.00	O
ATOM	3364	CB	TYR	B	848	1.842	0.546	43.729	1.00	18.82	C
ATOM	3365	CG	TYR	B	848	2.919	0.943	44.731	1.00	15.40	C
ATOM	3366	CD1	TYR	B	848	2.753	1.970	45.606	1.00	11.34	C
ATOM	3367	CD2	TYR	B	848	4.118	0.198	44.757	1.00	12.91	C
ATOM	3368	CE1	TYR	B	848	3.704	2.377	46.481	1.00	7.89	C
ATOM	3369	CE2	TYR	B	848	5.081	0.627	45.608	1.00	12.03	C
ATOM	3370	CZ	TYR	B	848	4.875	1.706	46.483	1.00	11.36	C
ATOM	3371	OH	TYR	B	848	5.890	2.063	47.369	1.00	9.44	O
ATOM	3372	N	ILE	B	849	-0.978	-0.988	42.487	1.00	21.21	N
ATOM	3373	CA	ILE	B	849	-2.265	-0.721	41.727	1.00	23.05	C
ATOM	3374	C	ILE	B	849	-3.382	-0.403	42.690	1.00	26.47	C
ATOM	3375	O	ILE	B	849	-4.124	0.545	42.631	1.00	25.33	O
ATOM	3376	CB	ILE	B	849	-2.426	-1.931	40.795	1.00	19.94	C
ATOM	3377	CG1	ILE	B	849	-1.159	-1.992	39.937	1.00	15.54	C
ATOM	3378	CG2	ILE	B	849	-3.770	-1.904	40.127	1.00	17.19	C
ATOM	3379	CD1	ILE	B	849	-1.372	-2.908	38.787	1.00	15.91	C
ATOM	3380	N	ARG	B	850	-3.567	-1.162	43.767	1.00	30.47	N
ATOM	3381	CA	ARG	B	850	-4.297	-1.073	45.000	1.00	28.54	C
ATOM	3382	C	ARG	B	850	-4.230	0.245	45.778	1.00	30.01	C
ATOM	3383	O	ARG	B	850	-5.208	0.733	46.384	1.00	29.39	O
ATOM	3384	CB	ARG	B	850	-3.713	-2.188	45.856	1.00	25.13	C
ATOM	3385	CG	ARG	B	850	-4.480	-3.489	45.783	1.00	25.66	C
ATOM	3386	CD	ARG	B	850	-4.301	-4.395	46.974	1.00	21.85	C
ATOM	3387	NE	ARG	B	850	-3.008	-4.963	47.228	1.00	22.00	N
ATOM	3388	CZ	ARG	B	850	-2.194	-6.007	47.010	1.00	21.87	C
ATOM	3389	NH1	ARG	B	850	-2.372	-7.125	46.238	1.00	16.56	N
ATOM	3390	NH2	ARG	B	850	-1.015	-5.815	47.725	1.00	16.89	N
ATOM	3391	N	GLU	B	851	-3.037	0.916	45.749	1.00	27.62	N
ATOM	3392	CA	GLU	B	851	-2.932	2.190	46.380	1.00	24.96	C
ATOM	3393	C	GLU	B	851	-3.655	3.162	45.513	1.00	24.96	C

FIG. 7 CONT'D

ATOM	3394	O	GLU	B	851	-4.063	4.145	46.089	1.00	25.56	O
ATOM	3395	CB	GLU	B	851	-1.517	2.708	46.658	1.00	25.87	C
ATOM	3396	CG	GLU	B	851	-1.412	3.779	47.807	1.00	21.42	C
ATOM	3397	CD	GLU	B	851	-1.865	3.071	49.095	1.00	18.95	C
ATOM	3398	OE1	GLU	B	851	-1.728	1.825	48.988	1.00	17.90	O
ATOM	3399	OE2	GLU	B	851	-2.341	3.644	50.073	1.00	16.47	O
ATOM	3400	N	LEU	B	852	-3.689	3.039	44.219	1.00	26.19	N
ATOM	3401	CA	LEU	B	852	-4.238	3.844	43.143	1.00	23.03	C
ATOM	3402	C	LEU	B	852	-5.781	3.813	43.129	1.00	24.94	C
ATOM	3403	O	LEU	B	852	-6.501	4.789	42.945	1.00	21.76	O
ATOM	3404	CB	LEU	B	852	-3.843	3.267	41.775	1.00	14.31	C
ATOM	3405	CG	LEU	B	852	-4.409	4.053	40.602	1.00	10.03	C
ATOM	3406	CD1	LEU	B	852	-3.918	5.477	40.607	1.00	2.02	C
ATOM	3407	CD2	LEU	B	852	-4.100	3.311	39.324	1.00	7.57	C
ATOM	3408	N	ILE	B	853	-6.258	2.575	43.430	1.00	26.93	N
ATOM	3409	CA	ILE	B	853	-7.670	2.473	43.855	1.00	26.99	C
ATOM	3410	C	ILE	B	853	-8.030	3.061	45.202	1.00	30.41	C
ATOM	3411	O	ILE	B	853	-9.130	3.579	45.316	1.00	32.41	O
ATOM	3412	CB	ILE	B	853	-8.129	1.023	43.850	1.00	23.00	C
ATOM	3413	CG1	ILE	B	853	-7.980	0.481	42.428	1.00	19.67	C
ATOM	3414	CG2	ILE	B	853	-9.505	0.773	44.388	1.00	20.02	C
ATOM	3415	CD1	ILE	B	853	-7.133	-0.749	42.809	1.00	23.56	C
ATOM	3416	N	LYS	B	854	-7.170	3.079	46.210	1.00	32.54	N
ATOM	3417	CA	LYS	B	854	-7.343	4.008	47.343	1.00	34.91	C
ATOM	3418	C	LYS	B	854	-7.331	5.515	47.028	1.00	37.36	C
ATOM	3419	O	LYS	B	854	-7.956	6.338	47.748	1.00	36.92	O
ATOM	3420	CB	LYS	B	854	-6.412	3.480	48.454	1.00	33.24	C
ATOM	3421	CG	LYS	B	854	-6.445	1.981	48.722	1.00	31.08	C
ATOM	3422	CD	LYS	B	854	-5.302	1.285	49.424	1.00	29.06	C
ATOM	3423	CE	LYS	B	854	-5.112	1.460	50.911	1.00	28.19	C
ATOM	3424	NZ	LYS	B	854	-3.954	0.812	51.612	1.00	25.68	N
ATOM	3425	N	ALA	B	855	-6.716	6.026	45.964	1.00	37.65	N
ATOM	3426	CA	ALA	B	855	-6.584	7.424	45.655	1.00	36.73	C
ATOM	3427	C	ALA	B	855	-7.764	7.967	44.855	1.00	35.80	C
ATOM	3428	O	ALA	B	855	-8.339	9.029	45.095	1.00	34.95	O
ATOM	3429	CB	ALA	B	855	-5.348	7.632	44.788	1.00	36.96	C
ATOM	3430	N	ILE	B	856	-8.110	7.173	43.875	1.00	36.18	N
ATOM	3431	CA	ILE	B	856	-9.317	7.258	43.092	1.00	35.82	C
ATOM	3432	C	ILE	B	856	-10.484	7.249	44.094	1.00	37.26	C
ATOM	3433	O	ILE	B	856	-11.369	8.048	43.987	1.00	33.81	O
ATOM	3434	CB	ILE	B	856	-9.672	6.105	42.119	1.00	34.46	C
ATOM	3435	CG1	ILE	B	856	-8.590	5.830	41.080	1.00	32.14	C
ATOM	3436	CG2	ILE	B	856	-11.082	6.397	41.505	1.00	31.81	C
ATOM	3437	CD1	ILE	B	856	-8.960	4.717	40.085	1.00	29.67	C
ATOM	3438	N	GLY	B	857	-10.448	6.355	45.083	1.00	39.83	N
ATOM	3439	CA	GLY	B	857	-11.345	6.313	46.204	1.00	41.12	C
ATOM	3440	C	GLY	B	857	-11.544	7.576	47.000	1.00	43.00	C
ATOM	3441	O	GLY	B	857	-12.511	7.709	47.749	1.00	41.73	O
ATOM	3442	N	LEU	B	858	-10.771	8.623	46.837	1.00	45.67	N
ATOM	3443	CA	LEU	B	858	-10.710	9.691	47.807	1.00	50.53	C
ATOM	3444	C	LEU	B	858	-11.769	10.737	47.463	1.00	56.36	C
ATOM	3445	O	LEU	B	858	-12.187	11.628	48.217	1.00	55.00	O
ATOM	3446	CB	LEU	B	858	-9.243	10.039	47.575	1.00	47.55	C
ATOM	3447	CG	LEU	B	858	-8.241	9.193	48.348	1.00	44.32	C
ATOM	3448	CD1	LEU	B	858	-6.841	9.589	47.917	1.00	43.80	C
ATOM	3449	CD2	LEU	B	858	-8.440	9.554	49.817	1.00	43.10	C
ATOM	3450	N	ARG	B	859	-12.199	10.617	46.200	1.00	62.89	N
ATOM	3451	CA	ARG	B	859	-12.898	11.645	45.450	1.00	70.18	C
ATOM	3452	C	ARG	B	859	-13.983	10.965	44.640	1.00	74.03	C
ATOM	3453	O	ARG	B	859	-15.193	11.106	44.868	1.00	75.14	O
ATOM	3454	CB	ARG	B	859	-12.023	12.423	44.459	1.00	71.62	C
ATOM	3455	CG	ARG	B	859	-11.467	13.743	44.925	1.00	74.53	C
ATOM	3456	CD	ARG	B	859	-10.388	14.398	44.067	1.00	76.86	C
ATOM	3457	NE	ARG	B	859	-9.775	15.436	44.861	1.00	80.82	N

FIG. 7 CONT'D

ATOM	3458	CZ	ARG	B	859	-8.634	16.059	44.990	1.00	83.66	C
ATOM	3459	NH1	ARG	B	859	-7.618	15.750	44.195	1.00	85.48	N
ATOM	3460	NH2	ARG	B	859	-8.404	16.995	45.918	1.00	84.56	N
ATOM	3461	N	GLN	B	860	-13.647	10.131	43.660	1.00	78.05	N
ATOM	3462	CA	GLN	B	860	-14.622	9.313	42.953	1.00	80.50	C
ATOM	3463	C	GLN	B	860	-15.255	8.319	43.943	1.00	83.01	C
ATOM	3464	O	GLN	B	860	-14.938	7.126	43.955	1.00	83.03	O
ATOM	3465	CB	GLN	B	860	-14.173	8.427	41.802	1.00	79.89	C
ATOM	3466	CG	GLN	B	860	-13.528	9.027	40.601	1.00	80.24	C
ATOM	3467	CD	GLN	B	860	-14.048	10.392	40.201	1.00	80.00	C
ATOM	3468	OE1	GLN	B	860	-14.864	10.405	39.271	1.00	79.80	O
ATOM	3469	NE2	GLN	B	860	-13.601	11.443	40.870	1.00	79.37	N
ATOM	3470	N	LYS	B	861	-16.198	8.860	44.716	1.00	85.20	N
ATOM	3471	CA	LYS	B	861	-17.184	8.028	45.389	1.00	85.81	C
ATOM	3472	C	LYS	B	861	-18.267	7.633	44.390	1.00	85.35	C
ATOM	3473	O	LYS	B	861	-19.333	8.205	44.386	1.00	86.36	O
ATOM	3474	CB	LYS	B	861	-17.736	8.756	46.610	1.00	85.25	C
ATOM	3475	CG	LYS	B	861	-18.263	10.141	46.335	1.00	85.71	C
ATOM	3476	CD	LYS	B	861	-18.396	10.976	47.599	1.00	86.81	C
ATOM	3477	CE	LYS	B	861	-17.107	11.703	47.979	1.00	87.23	C
ATOM	3478	NZ	LYS	B	861	-17.221	12.682	49.099	1.00	86.59	N
ATOM	3479	N	GLY	B	862	-17.991	6.732	43.466	1.00	85.36	N
ATOM	3480	CA	GLY	B	862	-19.038	5.847	42.941	1.00	85.34	C
ATOM	3481	C	GLY	B	862	-18.702	4.404	43.298	1.00	84.67	C
ATOM	3482	O	GLY	B	862	-18.173	4.055	44.359	1.00	84.76	O
ATOM	3483	N	VAL	B	863	-18.923	3.527	42.367	1.00	84.22	N
ATOM	3484	CA	VAL	B	863	-18.596	2.113	42.300	1.00	83.12	C
ATOM	3485	C	VAL	B	863	-18.548	1.810	40.785	1.00	82.60	C
ATOM	3486	O	VAL	B	863	-17.835	0.995	40.213	1.00	83.81	O
ATOM	3487	CB	VAL	B	863	-19.620	1.184	42.963	1.00	82.44	C
ATOM	3488	CG1	VAL	B	863	-21.046	1.403	42.485	1.00	81.87	C
ATOM	3489	CG2	VAL	B	863	-19.226	-0.280	42.768	1.00	82.57	C
ATOM	3490	N	VAL	B	864	-19.409	2.591	40.129	1.00	80.06	N
ATOM	3491	CA	VAL	B	864	-19.389	2.831	38.710	1.00	76.97	C
ATOM	3492	C	VAL	B	864	-18.387	3.918	38.345	1.00	74.96	C
ATOM	3493	O	VAL	B	864	-17.597	3.635	37.448	1.00	74.66	O
ATOM	3494	CB	VAL	B	864	-20.793	3.135	38.146	1.00	76.34	C
ATOM	3495	CG1	VAL	B	864	-21.117	4.602	37.961	1.00	74.67	C
ATOM	3496	CG2	VAL	B	864	-20.921	2.308	36.860	1.00	75.67	C
ATOM	3497	N	SER	B	865	-18.371	5.066	38.991	1.00	72.50	N
ATOM	3498	CA	SER	B	865	-17.421	6.125	38.681	1.00	70.18	C
ATOM	3499	C	SER	B	865	-15.976	5.690	38.904	1.00	67.71	C
ATOM	3500	O	SER	B	865	-15.047	5.632	38.094	1.00	67.11	O
ATOM	3501	CB	SER	B	865	-17.665	7.302	39.640	1.00	70.77	C
ATOM	3502	OG	SER	B	865	-16.461	8.016	39.911	1.00	72.05	O
ATOM	3503	N	SER	B	866	-15.738	5.328	40.161	1.00	64.10	N
ATOM	3504	CA	SER	B	866	-14.498	4.711	40.590	1.00	61.29	C
ATOM	3505	C	SER	B	866	-13.878	3.789	39.565	1.00	59.37	C
ATOM	3506	O	SER	B	866	-12.681	3.942	39.315	1.00	58.39	O
ATOM	3507	CB	SER	B	866	-14.790	3.914	41.875	1.00	61.09	C
ATOM	3508	OG	SER	B	866	-15.641	4.791	42.617	1.00	61.22	O
ATOM	3509	N	SER	B	867	-14.676	2.857	39.050	1.00	57.75	N
ATOM	3510	CA	SER	B	867	-14.244	1.872	38.067	1.00	56.34	C
ATOM	3511	C	SER	B	867	-13.801	2.566	36.790	1.00	55.94	C
ATOM	3512	O	SER	B	867	-12.720	2.275	36.279	1.00	57.38	O
ATOM	3513	CB	SER	B	867	-15.334	0.841	37.808	1.00	55.97	C
ATOM	3514	OG	SER	B	867	-14.921	-0.454	37.475	1.00	54.16	O
ATOM	3515	N	GLN	B	868	-14.564	3.514	36.309	1.00	53.04	N
ATOM	3516	CA	GLN	B	868	-14.388	4.091	34.983	1.00	50.26	C
ATOM	3517	C	GLN	B	868	-13.108	4.914	34.958	1.00	45.00	C
ATOM	3518	O	GLN	B	868	-12.270	4.815	34.081	1.00	41.45	O
ATOM	3519	CB	GLN	B	868	-15.660	4.879	34.659	1.00	54.27	C
ATOM	3520	CG	GLN	B	868	-17.047	4.271	34.677	1.00	57.89	C
ATOM	3521	CD	GLN	B	868	-18.183	5.015	33.963	1.00	60.87	C

FIG. 7 CONT'D

ATOM	3522	OE1	GLN	B	868	-18.999	4.494	33.132	1.00	61.66	O
ATOM	3523	NE2	GLN	B	868	-18.328	6.336	34.217	1.00	60.09	N
ATOM	3524	N	ARG	B	869	-12.962	5.736	36.004	1.00	39.89	N
ATOM	3525	CA	ARG	B	869	-11.720	6.349	36.437	1.00	33.57	C
ATOM	3526	C	ARG	B	869	-10.487	5.452	36.576	1.00	33.16	C
ATOM	3527	O	ARG	B	869	-9.516	5.798	35.932	1.00	32.10	O
ATOM	3528	CB	ARG	B	869	-11.829	7.063	37.785	1.00	24.04	C
ATOM	3529	CG	ARG	B	869	-10.689	8.062	37.775	1.00	16.50	C
ATOM	3530	CD	ARG	B	869	-10.997	9.279	38.619	1.00	11.39	C
ATOM	3531	NE	ARG	B	869	-10.288	10.375	38.151	1.00	14.00	N
ATOM	3532	CZ	ARG	B	869	-9.685	11.412	37.643	1.00	16.83	C
ATOM	3533	NH1	ARG	B	869	-10.274	11.984	36.595	1.00	16.43	N
ATOM	3534	NH2	ARG	B	869	-8.577	12.112	37.971	1.00	16.97	N
ATOM	3535	N	PHE	B	870	-10.469	4.368	37.301	1.00	33.73	N
ATOM	3536	CA	PHE	B	870	-9.469	3.339	37.147	1.00	36.35	C
ATOM	3537	C	PHE	B	870	-9.076	3.007	35.735	1.00	39.88	C
ATOM	3538	O	PHE	B	870	-7.900	2.992	35.424	1.00	40.26	O
ATOM	3539	CB	PHE	B	870	-9.797	1.976	37.806	1.00	33.18	C
ATOM	3540	CG	PHE	B	870	-8.607	1.063	37.940	1.00	30.32	C
ATOM	3541	CD1	PHE	B	870	-7.451	1.438	38.599	1.00	29.20	C
ATOM	3542	CD2	PHE	B	870	-8.615	-0.229	37.425	1.00	29.63	C
ATOM	3543	CE1	PHE	B	870	-6.385	0.569	38.693	1.00	27.05	C
ATOM	3544	CE2	PHE	B	870	-7.572	-1.103	37.481	1.00	26.07	C
ATOM	3545	CZ	PHE	B	870	-6.468	-0.678	38.136	1.00	26.44	C
ATOM	3546	N	TYR	B	871	-10.000	2.598	34.909	1.00	45.64	N
ATOM	3547	CA	TYR	B	871	-9.784	2.363	33.481	1.00	49.06	C
ATOM	3548	C	TYR	B	871	-9.076	3.540	32.795	1.00	47.42	C
ATOM	3549	O	TYR	B	871	-8.187	3.344	31.972	1.00	45.66	O
ATOM	3550	CB	TYR	B	871	-11.055	2.152	32.634	1.00	52.77	C
ATOM	3551	CG	TYR	B	871	-10.842	2.251	31.129	1.00	55.53	C
ATOM	3552	CD1	TYR	B	871	-10.258	1.152	30.502	1.00	57.62	CD2 C
ATOM	3553	CD2	TYR	B	871	-11.180	3.347	30.339	1.00	55.90	CD1 C
ATOM	3554	CE1	TYR	B	871	-10.009	1.101	29.151	1.00	58.38	CE2 C
ATOM	3555	CE2	TYR	B	871	-10.917	3.330	28.980	1.00	58.11	CE1 C
ATOM	3556	CZ	TYR	B	871	-10.345	2.201	28.379	1.00	59.00	C
ATOM	3557	OH	TYR	B	871	-10.120	2.178	27.001	1.00	58.68	O
ATOM	3558	N	GLN	B	872	-9.593	4.729	33.103	1.00	46.06	N
ATOM	3559	CA	GLN	B	872	-9.117	5.917	32.420	1.00	46.15	C
ATOM	3560	C	GLN	B	872	-7.665	6.222	32.811	1.00	44.06	C
ATOM	3561	O	GLN	B	872	-6.897	6.747	31.983	1.00	44.00	O
ATOM	3562	CB	GLN	B	872	-9.894	7.193	32.740	1.00	47.07	C
ATOM	3563	CG	GLN	B	872	-11.376	7.159	32.469	1.00	50.04	C
ATOM	3564	CD	GLN	B	872	-12.070	8.390	33.039	1.00	50.02	C
ATOM	3565	OE1	GLN	B	872	-12.386	8.402	34.233	1.00	48.18	O
ATOM	3566	NE2	GLN	B	872	-12.234	9.353	32.122	1.00	50.35	N
ATOM	3567	N	LEU	B	873	-7.352	5.938	34.103	1.00	39.32	N
ATOM	3568	CA	LEU	B	873	-6.052	6.433	34.544	1.00	33.09	C
ATOM	3569	C	LEU	B	873	-5.113	5.299	34.223	1.00	35.23	C
ATOM	3570	O	LEU	B	873	-3.994	5.715	33.896	1.00	37.26	O
ATOM	3571	CB	LEU	B	873	-6.202	6.865	35.932	1.00	24.69	C
ATOM	3572	CG	LEU	B	873	-7.019	8.089	36.247	1.00	19.19	C
ATOM	3573	CD1	LEU	B	873	-7.078	8.042	37.799	1.00	15.99	C
ATOM	3574	CD2	LEU	B	873	-6.335	9.316	35.665	1.00	14.96	C
ATOM	3575	N	THR	B	874	-5.565	4.067	34.187	1.00	36.04	N
ATOM	3576	CA	THR	B	874	-4.775	3.038	33.487	1.00	36.82	C
ATOM	3577	C	THR	B	874	-4.745	3.154	31.978	1.00	37.97	C
ATOM	3578	O	THR	B	874	-3.610	3.112	31.484	1.00	38.86	O
ATOM	3579	CB	THR	B	874	-5.076	1.617	33.994	1.00	32.96	C
ATOM	3580	OG1	THR	B	874	-6.316	1.162	33.527	1.00	31.32	O
ATOM	3581	CG2	THR	B	874	-5.349	1.618	35.487	1.00	32.15	C
ATOM	3582	N	LYS	B	875	-5.752	3.392	31.153	1.00	37.87	N
ATOM	3583	CA	LYS	B	875	-5.418	3.615	29.740	1.00	39.39	C
ATOM	3584	C	LYS	B	875	-4.430	4.759	29.516	1.00	37.88	C
ATOM	3585	O	LYS	B	875	-3.552	4.679	28.639	1.00	37.34	O

FIG. 7 CONT'D

ATOM	3586	CB	LYS	B	875	-6.679	3.817	28.901	1.00	41.43	C
ATOM	3587	CG	LYS	B	875	-6.546	3.712	27.374	1.00	39.92	C
ATOM	3588	CD	LYS	B	875	-6.025	2.309	27.095	1.00	39.90	C
ATOM	3589	CE	LYS	B	875	-6.186	1.843	25.663	1.00	37.84	C
ATOM	3590	NZ	LYS	B	875	-6.434	0.365	25.610	1.00	37.69	N
ATOM	3591	N	LEU	B	876	-4.505	5.855	30.226	1.00	35.39	N
ATOM	3592	CA	LEU	B	876	-3.513	6.891	30.166	1.00	35.28	C
ATOM	3593	C	LEU	B	876	-2.066	6.468	30.246	1.00	36.78	C
ATOM	3594	O	LEU	B	876	-1.183	7.039	29.623	1.00	38.74	O
ATOM	3595	CB	LEU	B	876	-3.666	7.884	31.323	1.00	31.12	C
ATOM	3596	CG	LEU	B	876	-3.079	9.244	31.061	1.00	28.60	C
ATOM	3597	CD1	LEU	B	876	-3.489	10.240	32.167	1.00	30.81	C
ATOM	3598	CD2	LEU	B	876	-1.580	9.379	31.124	1.00	28.74	C
ATOM	3599	N	LEU	B	877	-1.770	5.586	31.188	1.00	35.85	N
ATOM	3600	CA	LEU	B	877	-0.398	5.129	31.286	1.00	34.37	C
ATOM	3601	C	LEU	B	877	-0.102	4.153	30.183	1.00	34.61	C
ATOM	3602	O	LEU	B	877	1.012	4.132	29.694	1.00	34.86	O
ATOM	3603	CB	LEU	B	877	-0.182	4.622	32.671	1.00	32.78	C
ATOM	3604	CG	LEU	B	877	-0.257	5.496	33.918	1.00	31.20	C
ATOM	3605	CD1	LEU	B	877	-0.606	4.484	35.009	1.00	31.06	C
ATOM	3606	CD2	LEU	B	877	1.025	6.242	34.287	1.00	28.82	C
ATOM	3607	N	ASP	B	878	-1.065	3.399	29.715	1.00	36.11	N
ATOM	3608	CA	ASP	B	878	-1.024	2.453	28.604	1.00	36.25	C
ATOM	3609	C	ASP	B	878	-0.575	3.187	27.368	1.00	36.85	C
ATOM	3610	O	ASP	B	878	0.288	2.873	26.589	1.00	35.54	O
ATOM	3611	CB	ASP	B	878	-2.392	1.835	28.435	1.00	32.85	C
ATOM	3612	CG	ASP	B	878	-2.594	0.674	29.380	1.00	33.48	C
ATOM	3613	OD1	ASP	B	878	-1.748	0.032	30.042	1.00	30.98	O
ATOM	3614	OD2	ASP	B	878	-3.823	0.365	29.444	1.00	36.18	O
ATOM	3615	N	ASN	B	879	-1.229	4.330	27.251	1.00	38.40	N
ATOM	3616	CA	ASN	B	879	-1.037	5.189	26.105	1.00	39.28	C
ATOM	3617	C	ASN	B	879	0.294	5.897	26.032	1.00	41.73	C
ATOM	3618	O	ASN	B	879	0.724	6.337	24.948	1.00	44.37	O
ATOM	3619	CB	ASN	B	879	-2.216	6.143	25.979	1.00	34.95	C
ATOM	3620	CG	ASN	B	879	-3.519	5.427	25.559	1.00	32.33	C
ATOM	3621	OD1	ASN	B	879	-4.451	6.221	25.918	1.00	28.86	O
ATOM	3622	ND2	ASN	B	879	-3.448	4.226	24.904	1.00	24.79	N
ATOM	3623	N	LEU	B	880	1.058	6.063	27.066	1.00	41.28	N
ATOM	3624	CA	LEU	B	880	2.298	6.792	27.061	1.00	39.85	C
ATOM	3625	C	LEU	B	880	3.393	5.953	26.474	1.00	40.48	C
ATOM	3626	O	LEU	B	880	4.408	6.523	26.102	1.00	39.85	O
ATOM	3627	CB	LEU	B	880	2.365	6.995	28.563	1.00	40.39	C
ATOM	3628	CG	LEU	B	880	2.739	8.308	29.203	1.00	40.99	C
ATOM	3629	CD1	LEU	B	880	3.630	7.961	30.394	1.00	39.38	C
ATOM	3630	CD2	LEU	B	880	3.433	9.335	28.286	1.00	37.95	C
ATOM	3631	N	HIS	B	881	3.291	4.624	26.416	1.00	42.94	N
ATOM	3632	CA	HIS	B	881	4.360	3.848	25.782	1.00	46.16	C
ATOM	3633	C	HIS	B	881	4.646	4.444	24.426	1.00	46.80	C
ATOM	3634	O	HIS	B	881	5.653	5.079	24.142	1.00	46.79	O
ATOM	3635	CB	HIS	B	881	3.983	2.387	25.754	1.00	48.95	C
ATOM	3636	CG	HIS	B	881	3.952	1.884	27.182	1.00	52.42	C
ATOM	3637	ND1	HIS	B	881	3.109	0.866	27.592	1.00	53.64	N
ATOM	3638	CD2	HIS	B	881	4.664	2.272	28.266	1.00	53.12	C
ATOM	3639	CE1	HIS	B	881	3.288	0.627	28.867	1.00	54.92	C
ATOM	3640	NE2	HIS	B	881	4.240	1.475	29.288	1.00	54.98	N
ATOM	3641	N	ASP	B	882	3.666	4.354	23.541	1.00	45.53	N
ATOM	3642	CA	ASP	B	882	3.595	4.954	22.240	1.00	42.05	C
ATOM	3643	C	ASP	B	882	4.341	6.255	22.143	1.00	38.18	C
ATOM	3644	O	ASP	B	882	5.399	6.292	21.547	1.00	37.05	O
ATOM	3645	CB	ASP	B	882	2.101	5.202	22.085	1.00	45.80	C
ATOM	3646	CG	ASP	B	882	1.235	4.009	21.686	1.00	48.20	C
ATOM	3647	OD1	ASP	B	882	1.249	2.983	22.385	1.00	45.80	O
ATOM	3648	OD2	ASP	B	882	0.537	4.242	20.633	1.00	50.43	O
ATOM	3649	N	LEU	B	883	3.778	7.259	22.795	1.00	33.70	N

FIG. 7 CONT'D

ATOM	3650	CA	LEU	B	883	4.441	8.545	23.060	1.00	29.89	C
ATOM	3651	C	LEU	B	883	5.894	8.517	23.507	1.00	30.40	C
ATOM	3652	O	LEU	B	883	6.773	9.109	22.890	1.00	31.27	O
ATOM	3653	CB	LEU	B	883	3.706	9.162	24.223	1.00	23.40	C
ATOM	3654	CG	LEU	B	883	3.440	10.606	24.425	1.00	20.38	C
ATOM	3655	CD1	LEU	B	883	2.023	10.720	25.063	1.00	19.64	C
ATOM	3656	CD2	LEU	B	883	4.453	11.426	25.146	1.00	17.79	C
ATOM	3657	N	VAL	B	884	6.245	7.728	24.530	1.00	27.37	N
ATOM	3658	CA	VAL	B	884	7.641	7.521	24.827	1.00	24.64	C
ATOM	3659	C	VAL	B	884	8.434	7.043	23.639	1.00	24.56	C
ATOM	3660	O	VAL	B	884	9.609	7.484	23.490	1.00	21.41	O
ATOM	3661	CB	VAL	B	884	7.815	6.682	26.152	1.00	19.60	C
ATOM	3662	CG1	VAL	B	884	9.238	6.473	26.587	1.00	11.31	C
ATOM	3663	CG2	VAL	B	884	6.922	7.383	27.175	1.00	17.54	C
ATOM	3664	N	LYS	B	885	7.867	6.206	22.723	1.00	23.49	N
ATOM	3665	CA	LYS	B	885	8.714	5.548	21.750	1.00	23.18	C
ATOM	3666	C	LYS	B	885	9.209	6.493	20.690	1.00	24.90	C
ATOM	3667	O	LYS	B	885	10.174	6.347	19.987	1.00	24.80	O
ATOM	3668	CB	LYS	B	885	8.033	4.489	20.988	1.00	22.88	C
ATOM	3669	CG	LYS	B	885	8.773	3.762	19.893	1.00	19.36	C
ATOM	3670	CD	LYS	B	885	7.736	2.707	19.422	1.00	19.10	C
ATOM	3671	CE	LYS	B	885	8.468	1.971	18.269	1.00	20.56	C
ATOM	3672	NZ	LYS	B	885	8.508	0.518	18.595	1.00	21.99	N
ATOM	3673	N	GLN	B	886	8.460	7.542	20.645	1.00	27.56	N
ATOM	3674	CA	GLN	B	886	8.782	8.819	20.059	1.00	29.48	C
ATOM	3675	C	GLN	B	886	9.841	9.630	20.711	1.00	29.11	C
ATOM	3676	O	GLN	B	886	10.838	9.861	20.013	1.00	30.81	O
ATOM	3677	CB	GLN	B	886	7.442	9.576	20.107	1.00	30.54	C
ATOM	3678	CG	GLN	B	886	6.552	8.836	19.134	1.00	31.90	C
ATOM	3679	CD	GLN	B	886	5.235	9.568	18.895	1.00	33.96	C
ATOM	3680	OE1	GLN	B	886	5.227	10.787	19.139	1.00	32.26	O
ATOM	3681	NE2	GLN	B	886	4.355	8.659	18.402	1.00	32.97	N
ATOM	3682	N	LEU	B	887	9.765	10.068	21.960	1.00	25.94	N
ATOM	3683	CA	LEU	B	887	11.009	10.580	22.601	1.00	21.19	C
ATOM	3684	C	LEU	B	887	12.136	9.587	22.309	1.00	20.61	C
ATOM	3685	O	LEU	B	887	13.231	10.070	21.924	1.00	19.81	O
ATOM	3686	CB	LEU	B	887	10.772	11.020	24.055	1.00	13.98	C
ATOM	3687	CG	LEU	B	887	9.350	11.534	24.371	1.00	12.02	C
ATOM	3688	CD1	LEU	B	887	9.134	11.711	25.850	1.00	10.99	C
ATOM	3689	CD2	LEU	B	887	8.762	12.769	23.644	1.00	2.02	C
ATOM	3690	N	HIS	B	888	11.975	8.255	22.373	1.00	18.68	N
ATOM	3691	CA	HIS	B	888	13.128	7.391	22.421	1.00	17.95	C
ATOM	3692	C	HIS	B	888	14.109	7.402	21.259	1.00	16.56	C
ATOM	3693	O	HIS	B	888	15.372	7.523	21.143	1.00	2.76	O
ATOM	3694	CB	HIS	B	888	12.523	5.996	22.683	1.00	17.27	C
ATOM	3695	CG	HIS	B	888	12.561	5.611	24.165	1.00	17.40	C
ATOM	3696	ND1	HIS	B	888	12.189	4.346	24.617	1.00	14.19	N
ATOM	3697	CD2	HIS	B	888	12.925	6.357	25.296	1.00	12.75	C
ATOM	3698	CE1	HIS	B	888	12.230	4.329	25.904	1.00	9.27	C
ATOM	3699	NE2	HIS	B	888	12.715	5.446	26.253	1.00	7.29	N
ATOM	3700	N	LEU	B	889	13.459	7.000	20.168	1.00	17.67	N
ATOM	3701	CA	LEU	B	889	13.965	7.273	18.838	1.00	18.57	C
ATOM	3702	C	LEU	B	889	14.502	8.668	18.620	1.00	16.85	C
ATOM	3703	O	LEU	B	889	15.627	8.907	18.160	1.00	16.59	O
ATOM	3704	CB	LEU	B	889	12.709	6.983	17.995	1.00	17.20	C
ATOM	3705	CG	LEU	B	889	12.924	7.007	16.497	1.00	15.05	C
ATOM	3706	CD1	LEU	B	889	14.377	6.830	16.080	1.00	11.53	C
ATOM	3707	CD2	LEU	B	889	12.120	5.763	16.139	1.00	20.26	C
ATOM	3708	N	TYR	B	890	13.826	9.753	18.995	1.00	15.98	N
ATOM	3709	CA	TYR	B	890	14.273	11.144	18.988	1.00	15.80	C
ATOM	3710	C	TYR	B	890	15.619	11.279	19.679	1.00	15.92	C
ATOM	3711	O	TYR	B	890	16.407	11.984	19.129	1.00	13.21	O
ATOM	3712	CB	TYR	B	890	13.256	12.167	19.520	1.00	14.10	C
ATOM	3713	CG	TYR	B	890	13.679	13.612	19.309	1.00	16.01	C

FIG. 7 CONT'D

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ATOM   3714  CD1 TYR B 890      13.442  14.213  18.091  1.00 13.30      CD2  C
ATOM   3715  CD2 TYR B 890      14.322  14.406  20.283  1.00 16.52      CD1  C
ATOM   3716  CE1 TYR B 890      13.870  15.448  17.762  1.00 11.78      CE2  C
ATOM   3717  CE2 TYR B 890      14.724  15.681  19.943  1.00 18.15      CE1  C
ATOM   3718  CZ  TYR B 890      14.476  16.234  18.679  1.00 17.51           C
ATOM   3719  OH  TYR B 890      14.884  17.535  18.332  1.00 19.47           O
ATOM   3720  N   CYS B 891      15.709  10.594  20.821  1.00 16.14           N
ATOM   3721  CA  CYS B 891      16.793  10.649  21.695  1.00 15.40           C
ATOM   3722  C   CYS B 891      17.952   9.869  21.094  1.00 17.49           C
ATOM   3723  O   CYS B 891      19.048  10.572  20.952  1.00 14.73           O
ATOM   3724  CB  CYS B 891      16.289  10.299  23.108  1.00 11.12           C
ATOM   3725  SG  CYS B 891      17.726  10.264  24.275  1.00  4.51           S
ATOM   3726  N   LEU B 892      17.703   8.611  20.648  1.00 15.56           N
ATOM   3727  CA  LEU B 892      18.894   7.943  20.046  1.00 19.16           C
ATOM   3728  C   LEU B 892      19.425   8.673  18.791  1.00 20.63           C
ATOM   3729  O   LEU B 892      20.691   8.866  18.634  1.00 16.74           O
ATOM   3730  CB  LEU B 892      18.904   6.454  19.972  1.00 17.28           C
ATOM   3731  CG  LEU B 892      19.226   5.263  19.089  1.00 17.15           C
ATOM   3732  CD1 LEU B 892      20.531   4.535  19.209  1.00 15.20           C
ATOM   3733  CD2 LEU B 892      18.229   4.111  19.144  1.00 11.84           C
ATOM   3734  N   ASN B 893      18.527   9.225  17.965  1.00 18.95           N
ATOM   3735  CA  ASN B 893      19.020   9.980  16.819  1.00 19.32           C
ATOM   3736  C   ASN B 893      19.918  11.136  17.172  1.00 20.72           C
ATOM   3737  O   ASN B 893      20.949  11.450  16.555  1.00 20.23           O
ATOM   3738  CB  ASN B 893      17.830  10.413  15.909  1.00 15.23           C
ATOM   3739  CG  ASN B 893      17.606   9.343  14.786  1.00 14.40           C
ATOM   3740  OD1 ASN B 893      16.510   9.000  14.326  1.00 12.57           O
ATOM   3741  ND2 ASN B 893      18.742   8.728  14.372  1.00  2.74           N
ATOM   3742  N   THR B 894      19.611  11.838  18.288  1.00 20.30           N
ATOM   3743  CA  THR B 894      20.313  13.045  18.639  1.00 17.91           C
ATOM   3744  C   THR B 894      21.563  12.601  19.343  1.00 20.83           C
ATOM   3745  O   THR B 894      22.615  13.229  19.290  1.00 19.07           O
ATOM   3746  CB  THR B 894      19.343  13.820  19.502  1.00 16.77           C
ATOM   3747  OG1 THR B 894      18.105  14.068  18.853  1.00 13.25           O
ATOM   3748  CG2 THR B 894      19.894  15.150  19.967  1.00 16.02           C
ATOM   3749  N   PHE B 895      21.508  11.442  20.011  1.00 24.80           N
ATOM   3750  CA  PHE B 895      22.779  10.891  20.601  1.00 25.35           C
ATOM   3751  C   PHE B 895      23.770  10.547  19.519  1.00 24.13           C
ATOM   3752  O   PHE B 895      24.748  11.151  19.245  1.00 21.42           O
ATOM   3753  CB  PHE B 895      22.557   9.709  21.552  1.00 24.79           C
ATOM   3754  CG  PHE B 895      23.599   9.119  22.443  1.00 23.13           C
ATOM   3755  CD1 PHE B 895      24.119   9.826  23.556  1.00 21.85           C
ATOM   3756  CD2 PHE B 895      24.111   7.841  22.195  1.00 21.00           C
ATOM   3757  CE1 PHE B 895      25.090   9.191  24.329  1.00 20.63           C
ATOM   3758  CE2 PHE B 895      25.155   7.318  23.000  1.00 17.97           C
ATOM   3759  CZ  PHE B 895      25.636   7.955  24.079  1.00 14.91           C
ATOM   3760  N   ILE B 896      23.568   9.505  18.741  1.00 25.81           N
ATOM   3761  CA  ILE B 896      24.326   9.265  17.542  1.00 28.03           C
ATOM   3762  C   ILE B 896      24.699  10.466  16.714  1.00 29.22           C
ATOM   3763  O   ILE B 896      25.826  10.414  16.245  1.00 25.47           O
ATOM   3764  CB  ILE B 896      23.536   8.286  16.667  1.00 29.09           C
ATOM   3765  CG1 ILE B 896      22.961   7.116  17.494  1.00 28.07           C
ATOM   3766  CG2 ILE B 896      24.431   7.801  15.524  1.00 29.16           C
ATOM   3767  CD1 ILE B 896      21.851   6.432  16.736  1.00 26.31           C
ATOM   3768  N   GLN B 897      23.856  11.458  16.402  1.00 31.53           N
ATOM   3769  CA  GLN B 897      24.405  12.610  15.669  1.00 34.11           C
ATOM   3770  C   GLN B 897      24.907  13.785  16.479  1.00 35.24           C
ATOM   3771  O   GLN B 897      25.129  14.885  15.989  1.00 34.94           O
ATOM   3772  CB  GLN B 897      23.410  13.170  14.672  1.00 33.84           C
ATOM   3773  CG  GLN B 897      23.437  12.614  13.259  1.00 33.85           C
ATOM   3774  CD  GLN B 897      21.930  12.417  13.012  1.00 35.17           C
ATOM   3775  OE1 GLN B 897      21.659  11.216  12.864  1.00 35.65           O
ATOM   3776  NE2 GLN B 897      21.303  13.588  13.032  1.00 34.05           N
ATOM   3777  N   SER B 898      25.099  13.656  17.781  1.00 35.52           N
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FIG. 7 CONT'D

ATOM	3778	CA	SER	B	898	25.413	14.707	18.661	1.00	33.62	C
ATOM	3779	C	SER	B	898	26.624	15.509	18.289	1.00	33.45	C
ATOM	3780	O	SER	B	898	26.592	16.645	18.735	1.00	34.54	O
ATOM	3781	CB	SER	B	898	25.610	14.034	20.025	1.00	30.68	C
ATOM	3782	OG	SER	B	898	26.960	13.689	19.991	1.00	27.78	O
ATOM	3783	N	ARG	B	899	27.653	15.104	17.667	1.00	35.55	N
ATOM	3784	CA	ARG	B	899	28.832	15.874	17.364	1.00	40.38	C
ATOM	3785	C	ARG	B	899	28.697	16.707	16.062	1.00	41.20	C
ATOM	3786	O	ARG	B	899	29.448	17.609	15.721	1.00	39.68	O
ATOM	3787	CB	ARG	B	899	30.010	14.963	17.183	1.00	41.53	C
ATOM	3788	CG	ARG	B	899	30.935	14.437	18.207	1.00	46.23	C
ATOM	3789	CD	ARG	B	899	31.975	13.446	17.697	1.00	48.94	C
ATOM	3790	NE	ARG	B	899	32.859	12.751	18.597	1.00	50.88	N
ATOM	3791	CZ	ARG	B	899	33.457	13.053	19.734	1.00	53.48	C
ATOM	3792	NH1	ARG	B	899	33.325	14.235	20.386	1.00	54.28	N
ATOM	3793	NH2	ARG	B	899	34.249	12.089	20.232	1.00	52.21	N
ATOM	3794	N	ALA	B	900	27.763	16.289	15.242	1.00	40.51	N
ATOM	3795	CA	ALA	B	900	27.400	17.066	14.094	1.00	40.10	C
ATOM	3796	C	ALA	B	900	26.495	18.109	14.713	1.00	40.90	C
ATOM	3797	O	ALA	B	900	26.814	19.301	14.542	1.00	41.97	O
ATOM	3798	CB	ALA	B	900	26.870	16.263	12.943	1.00	38.11	C
ATOM	3799	N	LEU	B	901	25.529	17.737	15.535	1.00	39.70	N
ATOM	3800	CA	LEU	B	901	24.544	18.698	16.019	1.00	36.26	C
ATOM	3801	C	LEU	B	901	24.962	19.569	17.170	1.00	36.70	C
ATOM	3802	O	LEU	B	901	24.163	20.472	17.547	1.00	38.56	O
ATOM	3803	CB	LEU	B	901	23.158	18.120	16.394	1.00	31.70	C
ATOM	3804	CG	LEU	B	901	22.974	16.821	15.577	1.00	27.80	C
ATOM	3805	CD1	LEU	B	901	22.024	15.857	16.264	1.00	23.82	C
ATOM	3806	CD2	LEU	B	901	22.779	17.383	14.177	1.00	25.92	C
ATOM	3807	N	SER	B	902	26.143	19.394	17.711	1.00	37.08	N
ATOM	3808	CA	SER	B	902	26.665	20.193	18.823	1.00	36.73	C
ATOM	3809	C	SER	B	902	25.919	20.013	20.156	1.00	36.59	C
ATOM	3810	O	SER	B	902	25.928	20.979	20.933	1.00	35.55	O
ATOM	3811	CB	SER	B	902	26.660	21.714	18.596	1.00	34.96	C
ATOM	3812	OG	SER	B	902	27.826	22.087	17.931	1.00	33.22	O
ATOM	3813	N	VAL	B	903	25.282	18.849	20.320	1.00	35.85	N
ATOM	3814	CA	VAL	B	903	24.624	18.708	21.599	1.00	36.50	C
ATOM	3815	C	VAL	B	903	25.514	17.844	22.517	1.00	34.32	C
ATOM	3816	O	VAL	B	903	26.116	16.801	22.207	1.00	31.53	O
ATOM	3817	CB	VAL	B	903	23.206	18.200	21.488	1.00	38.53	C
ATOM	3818	CG1	VAL	B	903	22.579	18.173	22.890	1.00	39.84	C
ATOM	3819	CG2	VAL	B	903	22.210	18.967	20.633	1.00	38.60	C
ATOM	3820	N	GLU	B	904	25.690	18.382	23.721	1.00	30.70	N
ATOM	3821	CA	GLU	B	904	26.288	17.595	24.800	1.00	32.36	C
ATOM	3822	C	GLU	B	904	25.312	16.718	25.599	1.00	29.17	C
ATOM	3823	O	GLU	B	904	24.482	17.354	26.244	1.00	26.03	O
ATOM	3824	CB	GLU	B	904	27.074	18.395	25.865	1.00	34.89	C
ATOM	3825	CG	GLU	B	904	27.616	17.503	26.953	1.00	40.06	C
ATOM	3826	CD	GLU	B	904	29.083	17.081	27.044	1.00	44.95	C
ATOM	3827	OE1	GLU	B	904	29.830	17.256	26.003	1.00	45.53	O
ATOM	3828	OE2	GLU	B	904	29.572	16.554	28.149	1.00	43.13	O
ATOM	3829	N	PHE	B	905	25.478	15.386	25.516	1.00	25.00	N
ATOM	3830	CA	PHE	B	905	24.920	14.438	26.485	1.00	21.52	C
ATOM	3831	C	PHE	B	905	25.834	14.215	27.677	1.00	20.95	C
ATOM	3832	O	PHE	B	905	27.000	13.888	27.426	1.00	23.36	O
ATOM	3833	CB	PHE	B	905	24.686	12.961	25.989	1.00	15.44	C
ATOM	3834	CG	PHE	B	905	23.458	12.984	25.080	1.00	12.51	C
ATOM	3835	CD1	PHE	B	905	23.579	13.601	23.813	1.00	6.60	C
ATOM	3836	CD2	PHE	B	905	22.231	12.515	25.543	1.00	8.50	C
ATOM	3837	CE1	PHE	B	905	22.474	13.689	23.002	1.00	2.13	C
ATOM	3838	CE2	PHE	B	905	21.160	12.707	24.686	1.00	7.63	C
ATOM	3839	CZ	PHE	B	905	21.261	13.332	23.453	1.00	5.34	C
ATOM	3840	N	PRO	B	906	25.403	14.434	28.916	1.00	20.49	N
ATOM	3841	CA	PRO	B	906	26.150	14.071	30.092	1.00	18.71	C

FIG. 7 CONT'D

ATOM	3842	C	PRO	B	906	26.343	12.592	30.348	1.00	15.77	C
ATOM	3843	O	PRO	B	906	25.292	11.974	30.361	1.00	9.47	O
ATOM	3844	CB	PRO	B	906	25.380	14.685	31.289	1.00	17.26	C
ATOM	3845	CG	PRO	B	906	24.279	15.433	30.757	1.00	18.79	C
ATOM	3846	CD	PRO	B	906	24.136	15.070	29.282	1.00	20.13	C
ATOM	3847	N	GLU	B	907	27.511	12.105	30.712	1.00	17.16	N
ATOM	3848	CA	GLU	B	907	27.704	10.803	31.380	1.00	18.98	C
ATOM	3849	C	GLU	B	907	26.590	9.876	31.862	1.00	17.58	C
ATOM	3850	O	GLU	B	907	26.525	8.743	31.404	1.00	14.04	O
ATOM	3851	CB	GLU	B	907	28.658	10.838	32.596	1.00	17.80	C
ATOM	3852	CG	GLU	B	907	30.150	11.036	32.357	1.00	19.85	C
ATOM	3853	CD	GLU	B	907	31.021	10.130	33.288	1.00	22.12	C
ATOM	3854	OE1	GLU	B	907	31.153	8.886	33.145	1.00	13.68	OE2 O
ATOM	3855	OE2	GLU	B	907	31.534	10.917	34.217	1.00	23.70	OE1 O
ATOM	3856	N	MET	B	908	25.741	10.236	32.804	1.00	18.45	N
ATOM	3857	CA	MET	B	908	24.898	9.191	33.366	1.00	20.31	C
ATOM	3858	C	MET	B	908	23.875	8.830	32.313	1.00	22.17	C
ATOM	3859	O	MET	B	908	23.465	7.721	32.148	1.00	21.86	O
ATOM	3860	CB	MET	B	908	24.123	9.520	34.632	1.00	17.73	C
ATOM	3861	CG	MET	B	908	24.764	8.769	35.763	1.00	21.03	C
ATOM	3862	SD	MET	B	908	24.105	9.373	37.312	1.00	24.57	S
ATOM	3863	CE	MET	B	908	23.828	11.151	36.984	1.00	24.35	C
ATOM	3864	N	MET	B	909	23.240	9.882	31.808	1.00	26.09	N
ATOM	3865	CA	MET	B	909	22.311	9.888	30.701	1.00	24.74	C
ATOM	3866	C	MET	B	909	22.931	9.202	29.491	1.00	22.49	C
ATOM	3867	O	MET	B	909	22.238	8.336	29.103	1.00	17.32	O
ATOM	3868	CB	MET	B	909	21.999	11.352	30.455	1.00	25.60	C
ATOM	3869	CG	MET	B	909	20.635	11.879	30.907	1.00	24.09	C
ATOM	3870	SD	MET	B	909	20.003	12.624	29.404	1.00	19.42	S
ATOM	3871	CE	MET	B	909	19.178	11.161	28.851	1.00	22.30	C
ATOM	3872	N	SER	B	910	24.139	9.374	29.041	1.00	22.97	N
ATOM	3873	CA	SER	B	910	24.818	8.721	27.992	1.00	24.79	C
ATOM	3874	C	SER	B	910	24.819	7.218	28.173	1.00	26.58	C
ATOM	3875	O	SER	B	910	24.685	6.522	27.174	1.00	25.19	O
ATOM	3876	CB	SER	B	910	26.215	9.246	27.924	1.00	22.80	C
ATOM	3877	OG	SER	B	910	26.607	9.966	26.797	1.00	23.47	O
ATOM	3878	N	GLU	B	911	24.885	6.764	29.400	1.00	27.63	N
ATOM	3879	CA	GLU	B	911	25.036	5.414	29.892	1.00	27.87	C
ATOM	3880	C	GLU	B	911	23.754	4.612	29.716	1.00	24.73	C
ATOM	3881	O	GLU	B	911	23.799	3.591	29.053	1.00	20.20	O
ATOM	3882	CB	GLU	B	911	25.433	5.239	31.369	1.00	30.73	C
ATOM	3883	CG	GLU	B	911	24.910	4.323	32.429	1.00	36.24	C
ATOM	3884	CD	GLU	B	911	25.738	3.916	33.652	1.00	43.49	C
ATOM	3885	OE1	GLU	B	911	26.386	4.786	34.351	1.00	46.17	OE2 O
ATOM	3886	OE2	GLU	B	911	26.025	2.758	34.173	1.00	45.61	OE1 O
ATOM	3887	N	VAL	B	912	22.690	5.068	30.324	1.00	23.14	N
ATOM	3888	CA	VAL	B	912	21.398	4.495	30.063	1.00	23.46	C
ATOM	3889	C	VAL	B	912	21.064	4.435	28.586	1.00	23.40	C
ATOM	3890	O	VAL	B	912	20.307	3.587	28.164	1.00	25.19	O
ATOM	3891	CB	VAL	B	912	20.263	5.230	30.775	1.00	21.45	C
ATOM	3892	CG1	VAL	B	912	20.679	5.596	32.173	1.00	21.74	C
ATOM	3893	CG2	VAL	B	912	19.778	6.516	30.084	1.00	22.10	C
ATOM	3894	N	ILE	B	913	21.300	5.386	27.732	1.00	21.49	N
ATOM	3895	CA	ILE	B	913	21.002	5.468	26.345	1.00	20.13	C
ATOM	3896	C	ILE	B	913	21.700	4.367	25.571	1.00	23.00	C
ATOM	3897	O	ILE	B	913	21.143	3.666	24.729	1.00	22.70	O
ATOM	3898	CB	ILE	B	913	21.336	6.928	25.989	1.00	16.46	C
ATOM	3899	CG1	ILE	B	913	20.036	7.629	26.412	1.00	14.29	C
ATOM	3900	CG2	ILE	B	913	21.696	7.284	24.561	1.00	14.03	C
ATOM	3901	CD1	ILE	B	913	20.170	9.102	26.249	1.00	13.21	C
ATOM	3902	N	ALA	B	914	22.995	4.143	25.750	1.00	25.79	N
ATOM	3903	CA	ALA	B	914	23.780	3.200	25.004	1.00	27.23	C
ATOM	3904	C	ALA	B	914	23.312	1.846	25.509	1.00	29.96	C
ATOM	3905	O	ALA	B	914	23.121	1.033	24.611	1.00	32.65	O

FIG. 7 CONT'D

ATOM	3906	CB	ALA	B	914	25.268	3.144	25.248	1.00	24.52	C
ATOM	3907	N	ALA	B	915	23.262	1.745	26.810	1.00	30.74	N
ATOM	3908	CA	ALA	B	915	22.856	0.551	27.483	1.00	32.59	C
ATOM	3909	C	ALA	B	915	21.506	0.046	27.056	1.00	33.88	C
ATOM	3910	O	ALA	B	915	21.345	-1.158	27.210	1.00	36.83	O
ATOM	3911	CB	ALA	B	915	22.738	0.649	29.037	1.00	31.42	C
ATOM	3912	N	GLN	B	916	20.430	0.807	26.909	1.00	32.85	N
ATOM	3913	CA	GLN	B	916	19.169	0.097	26.762	1.00	31.20	C
ATOM	3914	C	GLN	B	916	18.302	0.629	25.623	1.00	28.91	C
ATOM	3915	O	GLN	B	916	17.312	-0.093	25.381	1.00	26.15	O
ATOM	3916	CB	GLN	B	916	18.425	-0.106	28.045	1.00	31.22	C
ATOM	3917	CG	GLN	B	916	19.073	-0.442	29.334	1.00	30.69	C
ATOM	3918	CD	GLN	B	916	19.442	-1.810	29.740	1.00	30.43	C
ATOM	3919	OE1	GLN	B	916	20.504	-2.110	30.314	1.00	29.99	O
ATOM	3920	NE2	GLN	B	916	18.421	-2.560	29.356	1.00	30.68	N
ATOM	3921	N	LEU	B	917	18.744	1.635	24.862	1.00	24.75	N
ATOM	3922	CA	LEU	B	917	17.675	2.314	24.128	1.00	22.71	C
ATOM	3923	C	LEU	B	917	17.429	1.722	22.751	1.00	24.08	C
ATOM	3924	O	LEU	B	917	16.346	1.500	22.135	1.00	20.08	O
ATOM	3925	CB	LEU	B	917	18.140	3.745	24.313	1.00	19.74	C
ATOM	3926	CG	LEU	B	917	16.950	4.652	24.176	1.00	18.83	C
ATOM	3927	CD1	LEU	B	917	15.889	4.226	25.208	1.00	18.41	C
ATOM	3928	CD2	LEU	B	917	17.356	6.077	24.097	1.00	17.63	C
ATOM	3929	N	PRO	B	918	18.536	1.302	22.131	1.00	26.23	N
ATOM	3930	CA	PRO	B	918	18.432	0.485	20.947	1.00	29.27	C
ATOM	3931	C	PRO	B	918	17.615	-0.746	21.285	1.00	33.99	C
ATOM	3932	O	PRO	B	918	16.500	-0.821	20.737	1.00	37.38	O
ATOM	3933	CB	PRO	B	918	19.814	0.279	20.455	1.00	26.37	C
ATOM	3934	CG	PRO	B	918	20.692	0.822	21.493	1.00	26.80	C
ATOM	3935	CD	PRO	B	918	19.929	1.461	22.599	1.00	25.13	C
ATOM	3936	N	LYS	B	919	18.008	-1.706	22.106	1.00	36.86	N
ATOM	3937	CA	LYS	B	919	17.218	-2.804	22.628	1.00	36.57	C
ATOM	3938	C	LYS	B	919	15.832	-2.421	23.097	1.00	33.26	C
ATOM	3939	O	LYS	B	919	14.954	-3.170	22.670	1.00	33.52	O
ATOM	3940	CB	LYS	B	919	17.997	-3.519	23.731	1.00	39.69	C
ATOM	3941	CG	LYS	B	919	17.492	-3.855	25.088	1.00	42.02	C
ATOM	3942	CD	LYS	B	919	16.821	-5.139	25.502	1.00	42.82	C
ATOM	3943	CE	LYS	B	919	17.748	-5.957	26.438	1.00	43.59	C
ATOM	3944	NZ	LYS	B	919	17.071	-7.148	27.024	1.00	40.83	N
ATOM	3945	N	ILE	B	920	15.513	-1.387	23.826	1.00	28.12	N
ATOM	3946	CA	ILE	B	920	14.123	-0.949	23.990	1.00	23.97	C
ATOM	3947	C	ILE	B	920	13.553	-0.502	22.651	1.00	22.28	C
ATOM	3948	O	ILE	B	920	12.419	-0.940	22.416	1.00	15.48	O
ATOM	3949	CB	ILE	B	920	13.977	0.102	25.100	1.00	21.67	C
ATOM	3950	CG1	ILE	B	920	14.632	-0.238	26.447	1.00	20.06	C
ATOM	3951	CG2	ILE	B	920	12.527	0.524	25.379	1.00	21.91	C
ATOM	3952	CD1	ILE	B	920	15.204	0.916	27.283	1.00	16.22	C
ATOM	3953	N	LEU	B	921	14.229	0.250	21.780	1.00	26.45	N
ATOM	3954	CA	LEU	B	921	13.514	0.672	20.539	1.00	32.29	C
ATOM	3955	C	LEU	B	921	13.349	-0.527	19.591	1.00	32.33	C
ATOM	3956	O	LEU	B	921	12.291	-0.596	18.990	1.00	32.64	O
ATOM	3957	CB	LEU	B	921	14.012	1.859	19.718	1.00	32.77	C
ATOM	3958	CG	LEU	B	921	14.022	3.299	20.264	1.00	34.41	C
ATOM	3959	CD1	LEU	B	921	15.148	4.207	19.784	1.00	30.85	C
ATOM	3960	CD2	LEU	B	921	12.714	4.035	19.948	1.00	33.18	C
ATOM	3961	N	ALA	B	922	14.192	-1.550	19.508	1.00	30.57	N
ATOM	3962	CA	ALA	B	922	13.961	-2.757	18.792	1.00	29.80	C
ATOM	3963	C	ALA	B	922	12.820	-3.585	19.325	1.00	29.13	C
ATOM	3964	O	ALA	B	922	12.646	-4.689	18.819	1.00	24.51	O
ATOM	3965	CB	ALA	B	922	15.203	-3.639	18.830	1.00	31.19	C
ATOM	3966	N	GLY	B	923	12.027	-3.139	20.266	1.00	31.21	N
ATOM	3967	CA	GLY	B	923	11.042	-3.908	20.980	1.00	33.85	C
ATOM	3968	C	GLY	B	923	11.466	-5.074	21.870	1.00	34.21	C
ATOM	3969	O	GLY	B	923	10.742	-6.006	22.246	1.00	32.50	O

FIG. 7 CONT'D

ATOM	3970	N	MET	B	924	12.723	-5.210	22.270	1.00	34.28	N
ATOM	3971	CA	MET	B	924	13.258	-6.391	22.849	1.00	36.26	C
ATOM	3972	C	MET	B	924	13.095	-6.281	24.362	1.00	37.24	C
ATOM	3973	O	MET	B	924	13.967	-6.757	25.096	1.00	36.76	O
ATOM	3974	CB	MET	B	924	14.731	-6.520	22.472	1.00	34.86	C
ATOM	3975	CG	MET	B	924	14.936	-7.130	21.131	1.00	36.40	C
ATOM	3976	SD	MET	B	924	14.407	-8.838	20.814	1.00	35.52	S
ATOM	3977	CE	MET	B	924	13.737	-8.529	19.158	1.00	33.64	C
ATOM	3978	N	VAL	B	925	12.087	-5.596	24.871	1.00	37.10	N
ATOM	3979	CA	VAL	B	925	11.507	-5.669	26.166	1.00	36.68	C
ATOM	3980	C	VAL	B	925	9.997	-5.895	26.316	1.00	37.55	C
ATOM	3981	O	VAL	B	925	9.203	-5.565	25.442	1.00	38.04	O
ATOM	3982	CB	VAL	B	925	11.848	-4.407	26.982	1.00	33.16	C
ATOM	3983	CG1	VAL	B	925	13.295	-3.968	26.844	1.00	33.55	C
ATOM	3984	CG2	VAL	B	925	10.801	-3.371	26.755	1.00	31.78	C
ATOM	3985	N	LYS	B	926	9.454	-6.418	27.399	1.00	37.96	N
ATOM	3986	CA	LYS	B	926	8.038	-6.570	27.623	1.00	38.82	C
ATOM	3987	C	LYS	B	926	7.334	-5.389	28.249	1.00	39.77	C
ATOM	3988	O	LYS	B	926	7.560	-4.912	29.381	1.00	38.98	O
ATOM	3989	CB	LYS	B	926	7.839	-7.735	28.599	1.00	38.45	C
ATOM	3990	CG	LYS	B	926	6.407	-8.288	28.730	1.00	36.89	C
ATOM	3991	CD	LYS	B	926	6.532	-9.766	29.158	1.00	36.58	C
ATOM	3992	CE	LYS	B	926	5.236	-10.509	29.410	1.00	35.88	C
ATOM	3993	NZ	LYS	B	926	5.203	-11.955	28.988	1.00	31.18	N
ATOM	3994	N	PRO	B	927	6.367	-4.899	27.469	1.00	38.92	N
ATOM	3995	CA	PRO	B	927	5.548	-3.836	28.094	1.00	41.01	C
ATOM	3996	C	PRO	B	927	4.485	-4.485	28.945	1.00	42.40	C
ATOM	3997	O	PRO	B	927	3.910	-5.521	28.622	1.00	42.98	O
ATOM	3998	CB	PRO	B	927	5.054	-2.969	26.966	1.00	37.90	C
ATOM	3999	CG	PRO	B	927	6.234	-3.050	26.046	1.00	37.23	C
ATOM	4000	CD	PRO	B	927	6.689	-4.487	26.088	1.00	37.12	C
ATOM	4001	N	LEU	B	928	4.265	-3.870	30.085	1.00	42.02	N
ATOM	4002	CA	LEU	B	928	3.200	-4.405	30.950	1.00	41.82	C
ATOM	4003	C	LEU	B	928	1.972	-3.654	30.529	1.00	42.29	C
ATOM	4004	O	LEU	B	928	1.940	-2.431	30.529	1.00	43.55	O
ATOM	4005	CB	LEU	B	928	3.659	-4.363	32.413	1.00	40.02	C
ATOM	4006	CG	LEU	B	928	5.105	-4.841	32.715	1.00	39.26	C
ATOM	4007	CD1	LEU	B	928	5.446	-4.729	34.194	1.00	38.81	C
ATOM	4008	CD2	LEU	B	928	5.514	-6.236	32.287	1.00	36.44	C
ATOM	4009	N	LEU	B	929	0.962	-4.303	29.998	1.00	43.59	N
ATOM	4010	CA	LEU	B	929	-0.232	-3.491	29.734	1.00	44.90	C
ATOM	4011	C	LEU	B	929	-1.357	-3.687	30.705	1.00	45.58	C
ATOM	4012	O	LEU	B	929	-1.714	-4.842	30.874	1.00	46.23	O
ATOM	4013	CB	LEU	B	929	-0.597	-3.873	28.330	1.00	45.22	C
ATOM	4014	CG	LEU	B	929	-0.003	-3.002	27.225	1.00	45.04	C
ATOM	4015	CD1	LEU	B	929	-0.207	-3.751	25.913	1.00	44.69	C
ATOM	4016	CD2	LEU	B	929	-0.656	-1.634	27.293	1.00	43.95	C
ATOM	4017	N	PHE	B	930	-1.910	-2.640	31.276	1.00	46.67	N
ATOM	4018	CA	PHE	B	930	-3.202	-2.733	31.948	1.00	48.98	C
ATOM	4019	C	PHE	B	930	-4.415	-3.123	31.112	1.00	53.77	C
ATOM	4020	O	PHE	B	930	-5.249	-3.841	31.685	1.00	52.14	O
ATOM	4021	CB	PHE	B	930	-3.399	-1.386	32.635	1.00	45.12	C
ATOM	4022	CG	PHE	B	930	-2.432	-1.023	33.718	1.00	40.19	C
ATOM	4023	CD1	PHE	B	930	-1.186	-0.509	33.427	1.00	38.37	C
ATOM	4024	CD2	PHE	B	930	-2.744	-1.164	35.061	1.00	38.15	C
ATOM	4025	CE1	PHE	B	930	-0.272	-0.193	34.418	1.00	35.25	C
ATOM	4026	CE2	PHE	B	930	-1.858	-0.795	36.067	1.00	34.55	C
ATOM	4027	CZ	PHE	B	930	-0.612	-0.306	35.745	1.00	33.36	C
ATOM	4028	N	HIS	B	931	-4.577	-2.717	29.841	1.00	59.84 >	N
ATOM	4029	CA	HIS	B	931	-5.659	-3.211	28.993	1.00	65.61 >	C
ATOM	4030	C	HIS	B	931	-5.335	-4.128	27.824	1.00	67.49 >	C
ATOM	4031	O	HIS	B	931	-4.379	-4.187	27.074	1.00	69.43 >	O
ATOM	4032	CB	HIS	B	931	-6.547	-2.069	28.431	1.00	67.38 >	C
ATOM	4033	CG	HIS	B	931	-7.009	-1.179	29.557	1.00	69.52 >	C

FIG. 7 CONT'D

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ATOM   4034  ND1 HIS B 931      -7.480  -1.721  30.745  1.00 70.22 >         N
ATOM   4035  CD2 HIS B 931      -7.026   0.169  29.691  1.00 69.24 >         C
ATOM   4036  CE1 HIS B 931      -7.792  -0.770  31.589  1.00 70.13 >         C
ATOM   4037  NE2 HIS B 931      -7.534   0.367  30.946  1.00 70.85 >         N
TER    4038
ATOM   4037  C1  R18 C   1      30.205  -8.891   6.181  1.00  8.30          C
ATOM   4038  C2  R18 C   1      29.548  -9.135   4.811  1.00  8.81          C
ATOM   4039  C3  R18 C   1      28.971 -10.534   4.787  1.00  9.13          C
ATOM   4040  O3  R18 C   1      29.052 -11.340   3.840  1.00  9.82          O
ATOM   4041  C4  R18 C   1      28.228 -10.856   6.001  1.00  4.19          C
ATOM   4042  C5  R18 C   1      28.019  -9.953   6.926  1.00  6.67          C
ATOM   4043  C6  R18 C   1      26.702  -9.744   7.635  1.00  6.77          C
ATOM   4044  C7  R18 C   1      27.172  -9.634   9.123  1.00  8.40          C
ATOM   4045  C8  R18 C   1      27.809  -8.234   9.173  1.00  9.54          C
ATOM   4046  C9  R18 C   1      29.010  -8.073   8.248  1.00 10.77          C
ATOM   4047  C10 R18 C   1      29.096  -9.005   7.243  1.00  8.06          C
ATOM   4048  C11 R18 C   1      30.019  -6.969   8.652  1.00  5.12          C
ATOM   4049  C12 R18 C   1      29.696  -6.197   9.664  1.00  4.01          C
ATOM   4050  C19 R18 C   1      29.999  -6.829  12.801  1.00  5.61          C
ATOM   4051  C13 R18 C   1      28.597  -6.445  10.657  1.00  4.73          C
ATOM   4052  C14 R18 C   1      28.239  -7.953  10.641  1.00  5.15          C
ATOM   4053  C15 R18 C   1      27.128  -8.054  11.694  1.00  4.93          C
ATOM   4054  C16 R18 C   1      27.326  -6.814  12.646  1.00  2.67          C
ATOM   4055  C17 R18 C   1      28.677  -6.170  12.267  1.00  2.10          C
ATOM   4056  C18 R18 C   1      27.485  -5.581   9.959  1.00  3.03          C
ATOM   4057  O17 R18 C   1      28.765  -4.842  12.729  1.00  4.49          O
ATOM   4058  C1  R18 D   2      14.001  16.978  30.267  1.00 17.24          C
ATOM   4059  C2  R18 D   2      13.456  16.649  31.689  1.00 17.47          C
ATOM   4060  C3  R18 D   2      11.985  16.738  31.622  1.00 17.75          C
ATOM   4061  O3  R18 D   2      11.215  17.129  32.431  1.00 20.12          O
ATOM   4062  C4  R18 D   2      11.323  16.255  30.411  1.00 21.17          C
ATOM   4063  C5  R18 D   2      12.007  15.672  29.404  1.00 19.86          C
ATOM   4064  C6  R18 D   2      11.294  14.757  28.459  1.00 15.57          C
ATOM   4065  C7  R18 D   2      12.144  14.872  27.187  1.00 13.21          C
ATOM   4066  C8  R18 D   2      13.590  14.436  27.350  1.00 12.65          C
ATOM   4067  C9  R18 D   2      14.245  15.398  28.314  1.00 13.89          C
ATOM   4068  C10 R18 D   2      13.484  15.934  29.273  1.00 18.09          C
ATOM   4069  C11 R18 D   2      15.692  15.717  28.177  1.00 10.62          C
ATOM   4070  C12 R18 D   2      16.466  15.282  27.194  1.00  9.38          C
ATOM   4071  C19 R18 D   2      16.677  16.177  24.293  1.00 16.12          C
ATOM   4072  C13 R18 D   2      15.793  14.407  26.160  1.00 10.03          C
ATOM   4073  C14 R18 D   2      14.324  14.804  26.024  1.00 10.05          C
ATOM   4074  C15 R18 D   2      13.933  14.136  24.693  1.00 12.08          C
ATOM   4075  C16 R18 D   2      15.249  14.106  23.810  1.00 11.44          C
ATOM   4076  C17 R18 D   2      16.328  14.708  24.723  1.00 12.42          C
ATOM   4077  C18 R18 D   2      16.142  12.886  26.296  1.00  2.02          C
ATOM   4078  O17 R18 D   2      17.667  14.197  24.766  1.00 15.32          O
ATOM   4079  O1  WAT W   1      27.787 -10.800   1.694  1.00  3.60          O
TER    4105
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FIG. 7 CONT'D

INTERNATIONAL SEARCH REPORT

Inte nal Application No
PCT/IB 01/00475

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 C07K14/72 G06F17/50

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 C07K G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
EPO-Internal, BIOSIS

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 97 21993 A (UNIV CALIFORNIA) 19 June 1997 (1997-06-19) page 11, line 10 -page 12, line 15; claim 10 --- -/--	1-5,7, 10,11, 13,14, 16-18, 30,31, 34-40

[X] Further documents are listed in the continuation of box C.

[X] Patent family members are listed in annex.

° Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier document but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
3 August 2001	21/08/2001

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL – 2280 HV Rijswijk Tel. (+31–70) 340–2040, Tx. 31 651 epo nl, Fax: (+31–70) 340–3016	Schwachtgen, J-L

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Form PCT/ISA/210 (second sheet) (July 1992)

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication,where appropriate, of the relevant passages	Relevant to claim No.
X	WILLIAMS SHAWN P ET AL: "Atomic structure of progesterone complexed with its receptor." NATURE (LONDON), vol. 393, no. 6683, 28 May 1998 (1998-05-28), pages 392-396, XP002173773 ISSN: 0028-0836 cited in the application	2,11, 36-38,40
Y	the whole document	1-5,7, 10,11, 34-38,40
Y	YONG E L ET AL: "Partial androgen insensitivity and correlations with the predicted three dimensional structure of the androgen receptor ligand-binding domain." MOLECULAR AND CELLULAR ENDOCRINOLOGY, vol. 13, no. 1, 13 February 1998 (1998-02-13), pages 41-50, XP001013088 ISSN: 0303-7207 cited in the application the whole document	1-5,7, 10,11, 34-38,40
A	GOTTLIEB BRUCE ET AL: "Update of the androgen receptor gene mutations database." HUMAN MUTATION, vol. 14, no. 2, 1999, pages 103-114, XP002173777 ISSN: 1059-7794 the whole document	
A	DATABASE BIOSIS 'Online! BIOSCIENCES INFORMATION SERVICE, PHILADELPHIA, PA, US; 1979 ZAVA D T ET AL: "ANDROGEN RECEPTOR ASSAY WITH TRITIATED METHYL TRIENOLONE R-1881 IN THE PRESENCE OF PROGESTERONE RECEPTORS" Database accession no. PREV197968033984 XP002173787 abstract & ENDOCRINOLOGY, vol. 104, no. 4, 1979, pages 1007-1012, EN ISSN: 0013-7227	
E	WO 01 27622 A (EINSPAHR HOWARD M ;SQUIBB BRISTOL MYERS CO (US); SACK JOHN S (US);) 19 April 2001 (2001-04-19) the whole document	1-4, 6-11, 13-18, 30,31, 34-40

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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication,where appropriate, of the relevant passages	Relevant to claim No.
P,X	MATIAS PEDRO M ET AL: "Structural evidence for ligand specificity in the binding domain of the human androgen receptor: Implications for pathogenic gene mutations." JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 275, no. 34, 25 August 2000 (2000-08-25), pages 26164-26171, XP002173776 ISSN: 0021-9258 the whole document	1-4, 6-18,30, 31,34-40
T	KLEBE GERHARD: "Recent developments in structure-based drug design." JOURNAL OF MOLECULAR MEDICINE (BERLIN), vol. 78, no. 5, 2000, pages 269-281, XP002173778 ISSN: 0946-2716	

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.2

Claims Nos.: 5, 19-29, 32, 33

Claim 5 is directed to a crystal of AR-LBD the secondary structure presented as SEQ ID No 2. However, a crystal structure cannot be described by a secondary structure and, in any case, SEQ ID No 2 is an empty primary nucleotide sequence file. A meaningful search on the subject-matter of claim 5 is therefore imposible (Article 6 PCT).

Claims 19-26, 32 and 33 are directed to LBD binding compounds, agonists and antagonists. However, no such compounds are defined in the application thereby rendering the subject-matter of said claims purely speculative and a mere statement of the result to be achieved. No meaningful search can be carried out for such "reach-through claims" whose scope is open-ended and unclear (Article 6 PCT). The same argument applies to claims 27-29.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.

INTERNATIONAL SEARCH REPORT

Information on patent family members

Inter ial Application No
PCT/IB 01/00475

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
WO 9721993 A	19-06-1997	AU 1821697 A	03-07-1997
		US 6236946 B	22-05-2001
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		JP 2000502086 T	22-02-2000
WO 0127622 A	19-04-2001	NONE	